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STRESS- AND CHEMISTRY-MEDIATED PERMEABILITY ENHANCEMENT/DEGRADATION IN STIMULATED CRITICALLY-STRESSED FRACTURES

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EXECUTIVE SUMMARY

This work has investigated the interactions between stress and chemistry in controlling the evolution of permeability in stimulated fractured reservoirs through an integrated program of experimentation and modeling. Flow-through experiments on natural and artificial fractures in Coso diorite have examined the evolution of permeability under paths of mean and deviatoric stresses, including the role of dissolution and precipitation. Models accommodating these behaviors have examined the importance of incorporating the complex couplings between stress and chemistry in examining the evolution of permeability in EGS reservoirs.

This document reports the findings of experiment [1,2] and analysis [3,4], in four sequential chapters.

[1] Results are reported for a long-term circulation test on a calcite-filled fracture in diorite from the Coso Geothermal Field, California. The fracture is circulated by DI water at 20°, then 60°, and then 90°C but under a near constant effective stress of 13 MPa. Through the initial stages of the test, at 20°C, the fracture aperture drops from an initial mean hydraulic aperture of 30 μm to 0.6 μm in the first 500 hours, before reaching a steady magnitude. This corresponds to a net reduction of ~ 4 orders of magnitude through the initial duration of the experiment, and under constant stress. As temperature is incremented, the average aperture further reduces, but a periodic change in aperture and hydraulic impedance is recorded under conditions of constant stress, temperature and pressure-controlled flow rate. The peak cyclic flow rate climbs rapidly to of the order of 20 times the steady magnitude, with a period of 6000 minutes, and is interpreted as periodic clogging and removal of mineral mass from the constricted and brecciated end of the sample. As the temperature is augmented to 90°C the flow rate continues to decrease, as a proxy for hydraulic aperture, ultimately reaching a final aperture of 1 μm and 0.03 cc/min. This low magnitude of ultimate permeability results, despite visible open voids within the calcite vein, with this response strongly conditioned by the evolving aqueous chemistry of the sample.

[2] The evolution of permeability in fractured rock as a function of effective normal stress, shear displacement, and damage remains a complex issue. In this contribution, we report on experiments in which rock surfaces were subject to direct shear under controlled pore pressure and true triaxial stress conditions while permeability was monitored continuously via flow parallel to the shear direction. Shear tests were performed in a pressure vessel under drained conditions on samples of novaculite (Arkansas) and diorite (Coso Geothermal field, CA). The sample pairs were sheared to 18 mm of total displacement at 5 $\mu\text{m}/\text{sec}$, at room temperature, and at effective normal stresses on the shear plane ranging from 5 to 20 MPa. Permeability evolution was measured throughout shearing via flow of distilled water from an upstream reservoir discharging downstream of the sample at atmospheric pressure. For diorite and novaculite, initial (pre-shear) fracture permeability is 0.5 to $1 \times 10^{-14} \text{ m}^2$, and largely independent of the applied effective normal stresses. These permeabilities correspond to equivalent hydraulic apertures of

15-20 μm . Because of the progressive formation of gouge during shear, the post-shear permeability of the diorite fracture drops to a final steady value of $0.5 \times 10^{-17} \text{ m}^2$. The behavior is similar in novaculite but the final permeability of $0.5 \times 10^{-16} \text{ m}^2$ is obtained only at an effective normal stress of 20 MPa.

[3] A method is introduced to couple the thermal (T), hydrologic (H), and chemical precipitation/dissolution (C) capabilities of TOUGHREACT with the mechanical (M) framework of FLAC^{3D} to examine THMC processes in deformable, fractured porous media. The combined influence of stress-driven asperity dissolution, thermal-hydro-mechanical asperity compaction/dilation, and mineral precipitation/dissolution alter the permeability of fractures during thermal, hydraulic, and chemical stimulation. Fracture and matrix are mechanically linked through linear, dual-porosity poroelasticity. Stress-dissolution effects are driven by augmented effective stresses incrementally defined at steady state with feedbacks to the transport system as a mass source, and to the mechanical system as an equivalent chemical strain. Porosity, permeability, stiffness, and chemical composition may be spatially heterogeneous and evolve with local temperature, effective stress and chemical potential. Changes in total stress generate undrained fluid pressure increments which are passed from the mechanical analysis to the transport logic with a correction to enforce conservation of fluid mass. Analytical comparisons confirm the capability of the model to represent the rapid, undrained response of the fluid-mechanical system to mechanical loading. We then focus on a full thermal loading/unloading cycle of a constrained fractured mass and follow irreversible alteration in *in-situ* stress and permeability resulting from both mechanical and chemical effects. In a companion paper [4] we examine a prototypical enhanced geothermal system (EGS) for changes in mechanical and transport properties, and outline in greater detail the strength of coupling between THMC mechanisms.

[4] This model is used to examine some of the dominant behaviors and permeability-altering mechanisms that may operate in naturally fractured media. Permeability and porosity are modified as fracture apertures dilate or contract under the influence of pressure solution, thermo-hydro-mechanical compaction/dilation, and mineral precipitation/dissolution. We examine a prototypical enhanced geothermal system (EGS) for the relative, temporal arrival of hydro-mechanical vs. thermo-mechanical vs. chemical changes in fluid transmission as cold (70°C) water is injected at geochemical disequilibrium within a heated reservoir (275°C). For an injection-withdrawal doublet separated by ~670m, the results demonstrate the strong influence of mechanical effects in the short term (several days), the influence of thermal effects in the intermediate term (<1 month at injection), and the prolonged and long-term (>1 year) influence of chemical effects, especially close to injection. In most of the reservoir, cooling enhances permeability and increases fluid circulation under pressure-drive. We observe thermo-mechanical driven permeability enhancement in front of the advancing thermal sweep, counteracted by the re-precipitation of minerals previously dissolved into the cool injection water. Near injection, calcite dissolution is capable of increasing permeability by nearly an order of magnitude, while precipitation of

amorphous silica onsets more slowly and can completely counteract this increase over the very long term (>10 years). For the reinjection of highly-silica-saturated water, amorphous silica is capable of drastic reduction in permeability close to the injection well. With combined action from all mechanisms, permeability change varies by two orders of magnitude between injection and withdrawal. We illustrate the importance of the coupling between reactive transport and geomechanics. Mineral behaviors alter fluid flow paths and, in so doing, change the characteristics of thermo-hydro-mechanical aperture changes, and vice versa. We show how each incurs changes in the system that fundamentally alter the evolutionary paths of reaction and chemical/mechanical deformation in a manner that mandates the accommodation of process couplings for the full THMC suite of interactions.

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1 CHAPTER 1: LONG-TERM EVOLUTION OF THE TRANSPORT PROPERTIES OF A FRACTURE FROM THE COSO GEOTHERMAL RESERVOIR

Abstract

Results are reported for a long-term circulation test on a calcite-filled fracture in diorite from the Coso Geothermal Field, California. The fracture is circulated by DI water at 20°, then 60°, and then 90°C but under a near constant effective stress of 13 MPa. Through the initial stages of the test, at 20°C, the fracture aperture drops from an initial mean hydraulic aperture of 30 μm to 0.6 μm in the first 500 hours, before reaching a steady magnitude. This corresponds to a net reduction of ~ 4 orders of magnitude through the initial duration of the experiment, and under constant stress. As temperature is incremented, the average aperture further reduces, but a periodic change in aperture and hydraulic impedance is recorded under conditions of constant stress, temperature and pressure-controlled flow rate. The peak cyclic flow rate climbs rapidly to of the order of 20 times the steady magnitude, with a period of 6000 minutes, and is interpreted as periodic clogging and removal of mineral mass from the constricted and brecciated end of the sample. As the temperature is augmented to 90°C the flow rate continues to decrease, as a proxy for hydraulic aperture, ultimately reaching a final aperture of 1 μm and 0.03 cc/min. This low magnitude of ultimate permeability results, despite visible open voids within the calcite vein, with this response strongly conditioned by the evolving aqueous chemistry of the sample. Analysis of the recovered data continues.

1.1 Introduction

Paths of stress, temperature, and chemical potential are known to strongly influence the evolution of the transport properties of rocks. This is especially true where the materials are fractured, and permeability is strongly coupled to relatively small changes in fracture apertures, that may in turn be driven by changes in stress or chemical potential. Data constraining the role of stress-mediated chemical effects in fractures are sparse, but are available at elevated temperatures ($>300^\circ\text{C}$) in granite [1], and at lower temperatures (50°C - 150°C) in tuff [2]. These are augmented by results for available composite aggregates of quartz [3], halite [4], calcite [5] and albite [6], at moderate temperatures (23°C - 150°C), and the same material suites at elevated temperatures and pressure [7]. The limited studies on fractures [1, 2, 8, 9, 10, 11] suggest an increased sensitivity of their transport properties to thermal, hydraulic, mechanical, and chemical processes, over porous medium flows. This is apparent even at temperatures as low as 100°C , where the mobile dissolved species in silica, the test duration is of order of a month [2, 3, 10], and where permeability may be reduced by a factor of 10^4 [2, 10].

Importantly, fracture permeabilities may either reduce or increase, in surprising ways, depending on the paths of stress or chemical potential. We illustrate this behavior through observations during flow –

thought tests on a sample of diorite core containing a natural calcite fracture from the Coso Geothermal Field in Coso, California.

1.2 Experimental Arrangement

Flow-through experiments are conducted and reported on fractured samples confined within an x-ray transparent cell to evaluate the influence of stress-mediated changes in dissolution and precipitation on the evolution in transport proprieties. Cylindrical samples containing a single fracture are confined within a flexible membrane and end-to-end flow tests completed, as illustrate in Fig. 1.

Three independent measurements are made to constrain the processes promoting the redistribution of mineral mass within the fracture: hydraulic flux, mineral mass flux, and volumetric imaging by x-ray CT. First, permeability is monitored continuously by prescribing flow rate and measuring pressure drop across the sample. Effective stresses are retained within a narrow range by controlling the upstream pressure. This measurement records permeability, and through this defines change in average aperture within the system [10]. Second, the net efflux of dissolved mineral mass is measured periodically to provide a record of net mass removal, and to correlate this whit observed changes in aperture, defined by the flow tests.

Fig. 1. Experimental arrangement showing confining cell and sample with axial fracture. Flow at prescribed flow-rate and pressure drop records permeability. Constraint on process is provided by measurement of dissolved mass efflux, and periodic scanning by x-ray CT. [11]

Finally, periodic non-destructive imaging by x-ray CT is used to view redistribution of mineral mass within the heated sample, as illustrated in figure 2. X-ray CT records changes in density within the sample as a proxy for mineral removal or redistribution, with the scanner used in this study capable of resolving down to $\sim 1/1000$ th of the diameter of the sample. For sample diameters of 3-5 cm used in the following study, the minimum voxel size scales to the order of 30-50 μm . This resolution is at the limits of utility in defining mass redistribution – it is adequate to define mass redistribution in samples of sandstone and limestone, but not for the relatively tighter fracture in novaculite.

The scanner used is an industrial third-generation microCT machine in the Center for Quantitative imaging at Penn State. The sample was scanned under confining stress through the X-ray transparent vessel. Complete 3-D volume scans were taken at the start and the end of the experiment, with additional partial scans during the experiment. Each full scan consists of X-ray absorption values of a $1024 \times 1024 \times 1150$ of the volume elements (voxels) that make up the sample. A commercial software package was used to extract the fracture volume from the rest of the sample. This is done by setting a threshold that separates the empty voxels of the fracture network from solid-filled voxels of the adjacent rock matrix. A percolation algorithm was then applied to the fracture network to determine connectivity between different portions of the fracture network. Given quantitative compatibility between image sets, the same procedure is applied to data taken before and after the experiment. Comparison of the two fracture networks allows comparison of the changes that have occurred with observed changes hydraulic properties.

These measurements provide unusual constraint on the evolving processes. Importantly, they allow the source of dissolved components to be determined: we need to discriminate whether the source is from free-face dissolution of the fracture wall, or from stress-mediated dissolution at contacting asperities. This distinction is crucial since these two mechanisms impart opposite effects in the sense of permeability change, under net dissolution: free-face dissolution increases permeability, and pressure solution reduces permeability.

1.3 Experimental Observations

Experimental observations record the redistribution of mineral mass within the sample through imaging, through the proxy of hydraulic response, and through measurements of the dissolved chemical efflux. The concurrent resolution of these three signals, adds constraint to the dominant processes which control the evolution of the mechanical and chemical response of fractures. Changes in aperture may be followed through imaging, through the reduction of the hydraulic aperture, and through measurement of the mass lost within the sample, also reduced to an equivalent change in aperture. These ensemble signals are described in the following.

Fig. 2. (a) Image of Coso core showing fracture infilled with calcite vein material, and voids. CT Images of the Coso core prior to circulation of fluid. (b) Face-on view, and (c) View of fracture rotated by 90° .

Fig. 3. Post-circulation images color-coded for connected porosity. The two colors denote disconnected fracture void volumes: (a) 90° rotated, (b) Front-on view, (c) Close-up of disconnected portion of the fracture.

1.3.1 Imaging

The experiment is completed on a core sample of diorite from a depth of 200 m above the Coso Geothermal Field. The sample contains a single through-going vein of calcite with multiple large tabular voids, as illustrated in Fig. 2(a). X-ray CT imaging of the core was completed pre- and post-experiment. The imaging shows the main conductive feature of the core – the central calcite vein containing numerous large tabular voids. These large voids occupy about 10% of the fracture volume, as illustrated in Figs. 2 (b) and (c), showing both the large voids and the smaller-aperture connected porosity. At the completion of the experiment, re-scanning notes changes in connectivity within the sample. The discrimination of connected porosity is a strong function of the threshold selected for the scanning – and not absolute. However, scanning is able to suggest that the large changes in permeability, witnessed in the later hydraulic results, occur as a result of necking-off of the fracture. At a particular CT threshold, the connected porosity divides into two distinct portions, as evident in Figs. 3(a) and 3(b). The constricted

transport pathway is strongly defined, involving a volume of a few voxels, as illustrated in the close-up of Fig. 3(c). Clearly, since the sample is always hydraulically connected, there is a void connection at this point, but it is severely constricted.

1.3.2 Hydraulic Behavior

The evolution of the fracture aperture is the second signal which may be followed with the progress of the experiment. The equivalent hydraulic aperture, b , is related to the recorded flow rate, Q and the pressure drop, dp , measured over the sample length, dl , as:

$$Q = d \cdot \frac{b^3}{12\mu} \cdot \frac{dp}{dl} \quad (1)$$

where d is the diameter of the cylindrical sample with a diametral fracture. This allows aperture to be used as a proxy for average change in the transport characteristics, as a common reference between imaging and inferred changes in transport characteristics due to precipitation and dissolution. The progress of aperture change measured from the hydraulic response is shown in Figure 3, for an experiment conducted at a constant effective stress of 13 MPa and at incremented temperatures of 20°, 60°, and 90°C.

The response shows a rapid reduction in aperture from 30µm under initial ambient stress and at 20°C to less than 1µm as the flow-through experiment continues, as illustrated in Fig. 4(a). After this initial closure in the first 100 hours, which never recovers, the aperture remains roughly constant in aperture, except for monotonic peaks and crests in calculated aperture which correlated with spikes in flow rate, for the experiment conducted under controlled pressure drop. These spikes in pressure appear to be in response to the plugging and then clearing of the fracture flow path. The post blockage episodes exhibit elevated mass concentrations, as illustrated in Fig. 4(b). This coherence in the signal suggests that fluid is locked behind an obstruction within the reservoir of the fracture void, before the blockage is cleared. This implicates precipitation or the obstruction by a mechanical blockage as causing this obstruction. The regular and repeating periodic nature of the blockage and purging signal suggests a characteristic response of the system, and favors control by precipitation, rather than by the random bridging by a trapped particle.

Fig. 4. (a) Change in hydraulic aperture with test duration together with mass concentrations of major ions. (b) Change in concentration of major ions with flow rate. Injection at 20°, 60°, and 90°C.

1.3.3 Chemical Behavior

Continuous measurements of the dissolved mass removed from the sample allow the cumulative mass removed to be evaluated. For a mass M removed in a given time interval, the equivalent change in aperture may be evaluated from the density of the dissolved mineral, ρ and the presumed surface area of removal, A_c , as $\Delta b = MA_c / \rho$. The mass removed is recovered from the product of volumetric flow rate, Q , and mass concentration, c , as $M = Qc$.

Where the system is far from equilibrium, and net dissolution prevails, net reduction in aperture suggests that mineral mass is being removed from the ridging asperities, and where aperture increases, then removal from the exposed free faces prevails. In each case, the active area of interest will be the asperity contact area, or the free face area, respectively.

These characterizations may be used to follow the cumulative mass removed from the fracture with time, as illustrated in Fig 5. The total mass removed from all sources over the 4000 hour-long experiment total 100mg from all sources. Of this the principal component is sodium accounting for 84% of the total.

Paradoxically, the signal for cumulative mass removed is not consistent with the aperture change. The aperture change occurs very early within the experiment, and is complete within the first 100 hours. However, mass continues to be removed from the fracture, and without any apparent change on the hydraulic response. This is apparent, even as temperatures are augmented with the progress of the experiment.

Fig. 5. Change in aperture determined from measured change in dissolved mass removed.

1.3.4 Process-Based Interpretations

Principal observations for this experiment are that despite continuous net dissolution throughout, the transmissive aperture of the fracture decreases, throughout. This could infer the removal of material from beneath bridging asperities, under the action of pressure dissolution, as has been implicated elsewhere [9; 10]. The rates of mass removal are of the same order as the rate of change in fracture aperture, as illustrated in Fig. 6. For removal of mass from a contact area of 20% of the total fracture area, results in a $\sim 30\mu\text{m}$ change in aperture, close to that recorded throughout the duration of the experiment. However, the timing of this removal is not congruent with the observed change in aperture, as recorded from the

hydraulic signal. To reconcile this mismatch in hydraulic and chemical observations, we consider a model of asperity crushing driven by local stresses at the asperity contacts. In this, the locally elevated stresses are able to fracture the calcite layer separating the asperity walls. This results in a rapid reduction in aperture as the material crushes, as illustrated in Fig. 7(a). This comminution results in elevated rates of mass dissolution (Fig. 7(b)) but with negligible reduction in aperture, due to an underlying asperity structure. This elevation in dissolution rates is reflected in the elevated mass removal rate recorded in the first portion of the experiment at 20°C. At the incrementing of temperature, this dissolution rate is sequentially elevated. This suggests that new fracturing is initiated with the addition of each temperature increment, possibly due to a slight reduction in the critical stress for pressure solution to begin, as illustrated in Fig. 8, although this suggests much smaller contact areas than those suggested by the chemical dissolution record.

Fig. 6. Changes in aperture produced for various contact area ratios of the contacting fracture.

Fig. 7. Change in critical stress with temperature for the experimental temperature of 20°, 60°, and 90°C.

Fig. 8. Process model of change in aperture with applied stress.

1.4 Discussion and Conclusions

Preliminary results are shown for changes in permeability which result from the circulation of reactive fluids within fractures. The change in aperture is severe, resulting in a change from 30 μ m to 1 μ m in the first 100 hours of the experiment, corresponding to a reduction in permeability of over three orders of magnitude.

Although the measured change in equivalent aperture, recovered from the hydraulic measurements, are of the same order as the cumulative mineral mass removed, the events are not coherent. The hydraulic change occurs rapidly, although the removal of mineral mass continues near continuously throughout the experiment. A preliminary model is suggested which honors these observations. This comprises the crushing of contacting asperity contacts, leaving crushed vain material with increased surface area for dissolution. This gives an elevated dissolution signature immediately post-crushing, which then drops with time. This behavior is observed in the response.

Although preliminary, these observations note the important influence of chemistry on the mechanical and transport properties of rocks, and in particular on the sensitivity of fractures to these effects.

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2 CHAPTER 2: THE INFLUENCE OF SHEAR AND DEVIATORIC STRESS ON THE EVOLUTION OF PERMEABILITY IN FRACTURED ROCK

Abstract

The evolution of permeability in fractured rock as a function of effective normal stress, shear displacement, and damage remains a complex issue. In this contribution, we report on experiments in which rock surfaces were subject to direct shear under controlled pore pressure and true triaxial stress conditions while permeability was monitored continuously via flow parallel to the shear direction. Shear tests were performed in a pressure vessel under drained conditions on samples of novaculite (Arkansas) and diorite (Coso Geothermal field, CA). The sample pairs were sheared to 18 mm of total displacement at 5 $\mu\text{m}/\text{sec}$, at room temperature, and at effective normal stresses on the shear plane ranging from 5 to 20 MPa. Permeability evolution was measured throughout shearing via flow of distilled water from an upstream reservoir discharging downstream of the sample at atmospheric pressure. For diorite and novaculite, initial (pre-shear) fracture permeability is 0.5 to $1 \times 10^{-14} \text{ m}^2$, and largely independent of the applied effective normal stresses. These permeabilities correspond to equivalent hydraulic apertures of 15-20 μm . Because of the progressive formation of gouge during shear, the post-shear permeability of the diorite fracture drops to a final steady value of $0.5 \times 10^{-17} \text{ m}^2$. The behavior is similar in novaculite but the final permeability of $0.5 \times 10^{-16} \text{ m}^2$ is obtained only at an effective normal stress of 20 MPa.

2.1 Introduction

Fluid flow and transport in fracture networks in rocks are relevant to a broad variety of scientific and industrial problems and processes, and have received considerable attention [1]. Most rock masses contain complex, interconnected networks of fractures with rough boundaries and breccia or, in some cases, gouge. Because of their high transmissivity, fractures are often conduits for fluid flow and transport; and their presence is critical in the recovery of hydrocarbons and geothermal fluids, and in mediating the evolution of fault zones and hydrothermal deposits.

Rocks and soils typically contain pores and fractures with a complex distribution of sizes and shapes [2,3]. Flow and transport of fluids in such porous media occurs not only through the microscopic pores, but also through fractures, which are typically much larger than the pores. Much effort has been expended to characterize the geometry of natural fracture systems as a precursor to defining their mechanical and transport properties [4].

For example, the orientation and intensity of fracturing in the subsurface of fracture-controlled geothermal fields are detected by measuring the fast-shear wave polarization and time delay from local

micro earthquakes [5, 6, 7, 8, 9; 10]. Also, fracture filling and fluid properties are related to fracture compliances and may be inferred from seismic data [11, 12, 13].

Fracture apertures and fracture connectivity together control the transport properties of fractured rocks, although the former is difficult to infer either directly or indirectly from seismic data. However, it has been argued that shear-wave anisotropy is sensitive to the fracture aspect ratio defined as the ratio of fracture aperture to length and therefore is related to the ambient stress field in the crust [4].

Moreover there have been many attempts to correlate the elastic (mechanical) and hydraulic (transport) properties of fractured rock [1,14-17]. These correlations are not always straightforward, and can sometimes be enigmatic, with the result that the inversion of seismic data for hydraulic transport properties is complex and must be done with care [18].

In summary, although there has been considerable success in the seismic characterization of natural fractures, it remains difficult to quantify several fundamental factors, including fracture density, shape, aperture, and connectivity. These are important initial conditions for hydrologic models, which underscores the difficulty of evaluating the evolution of fracture properties with stress history. A key purpose of this paper is to provide direct information on the relationship between fracture properties.

Recently other studies investigating the evolution of the mechanical and transport properties of fractured rocks relate the mechanical effects of crack formation, dilation, and closure, with chemical effects of stress mediated dissolution and precipitation. In particular, these effects are common either for micro cracks [19] or faults [20,21]. The temperature and chemical potential of the circulating fluid also has a significant influence on the evolution of strength and permeability. This is apparent in observations at high temperatures in granite [22], and at lower temperatures in tuff [23] and in composite aggregates of quartz [24], halite [25], calcite[26] and albite [27,28].

Although reactive transport is somewhat well defined in granular aggregates [29,30] the relevant processes in fractured systems are poorly understood. For this reason, predicting changes in transport parameters due to pressure solution and the circulation of geothermal fluids remains a complex task, [22,31-34].

In this study we investigated the changes in permeability of artificial fractures in novaculite and diorite under a range of conditions. In particular we focus on the effects that shear stress and triaxial stress state exert on mechanical (compaction and dilation), hydraulic (permeability) and chemical (advection and dissolution phenomena) behaviors of the fractures.

2.2 Experimental Method

Experiments were conducted on mated smooth-faced rock samples confined under normal stress. The samples were sheared, and concurrent measurements of strength and permeability were made as a function of shear offset under isothermal conditions. We begin by documenting the capabilities of the system, the experimental procedure, and key features of data analysis.

2.2.1 Experimental Equipment

The equipment consists of a steel pressure vessel of dimensions $\sim 50 \times 50 \times 40$ cm, capable of applying confining and pore pressures of up to 70 MPa and independent applied biaxial-stresses in excess of 300 MPa. The vessel has removable doors to allow access to the sample during set-up (Fig. 1). In our experiments, samples are placed within this pressure vessel (Fig. 2) and are loaded biaxially by servo-controlled hydraulic rams. Normal and shear stresses on the fracture surface are applied directly via loading pistons and are measured to a resolution of 0.01 MPa. Relative displacements parallel and perpendicular to the fracture plane are recorded by two DCDTs, accurate to 0.1 μm , mounted on the loading rams external to the pressure vessel. The sample assembly is jacketed within a thin, flexible latex membrane (Fig. 2) and confining pressure is applied via the surrounding fluid. True tri-axial loading conditions are achieved via the two loading pistons and the confining pressure, each of which is servo-controlled independently (Fig. 1). In addition, two high-precision servo-controlled pressure intensifiers are used to apply pore fluid pressure to the sample.

We conducted experiments on paired prismatic rock plates 11-12 mm thick, 45 mm wide and 50 and 70 mm long, respectively (Fig. 2). Direct shear is accomplished by motion of the longer block relative to a stationary shorter block, with constant nominal contact area of 45 mm $\times$ 50 mm (Fig. 2). The forcing platens have fittings and fluid delivery ports for pore fluid access to the sample. The sample assembly is first loaded in the fracture-normal direction and then subject to confining pressure and vertical load to apply shear stress on the fracture plane. A roller-way bearing allows a double-direct shear configuration to be used as single-direct shear (Figs. 1 and 2).

Fig. 1. Equipment arrangement showing pressure vessel, pressure intensifiers, schematic of plumbing arrangement, and experiment configuration for direct shear of the fracture samples.

Fig. 2. (a) Sample set up showing jacket, sealing collars, fluid piping internal to the pressure vessel, flow path and line-source fluid distribution at top and bottom of fracture surface, access, sample holders, and roller bearing for direct shear in the double-direct shear configuration. (b) Photo of novaculite sample and schematic of sample geometry showing main dimensions: A_T is the area perpendicular to the flow direction, which is used in Darcy's law.

In our experiments a load is applied at the top of the longer forcing block, producing shear relative to the static side block (Figs. 1 and 2). Pore fluid is supplied along a line source at the top and base of the static load platen (Fig. 2), allowing either uniform or differential fluid pressures to be applied along the shear surface. This fluid input is controlled by upstream and downstream reservoirs (Fig. 1). The jacketing

system has been configured to guarantee a seal on the sample during the large relative displacements sustained during these shear experiments. It comprises two layers of latex tubing (diameter: 7 cm and length: 15 cm) surrounding the sample, sealed by two rubber o-rings constricted by two aluminum collars (54.5×70 mm and 54.5×90 mm). Between the latex layer and the surfaces of the sample another rubber layer, which is 3-mm thick, is used to protect the jackets from puncturing when a confining pressure is applied (Fig. 2).

2.2.2 Experimental Procedure

The faces of the rock plates are surface-ground to be both square and parallel. The contact surfaces are then roughened by polishing with 60# grit for approximately 10 minutes and finally rinsed with distilled water and jacketed. Samples are positioned in the pressure vessel, then normal stress is applied and pore pressure intensifiers are connected, after which the vessel doors are closed and sealed. The pressure vessel is then filled with the confining fluid (XCEL THERM® 600 oil from Radco Industries). Permeability evolution is measured continuously before, during and after the shear test via flow of distilled water from an upstream reservoir that discharges downstream at atmospheric pressure. The discharge fluid is collected for chemical analysis using mass spectrometry (ICP-MS). The shear test begins after the flow rate has reached steady state.

Permeability is calculated from Darcy's law according to:

$$k = \frac{Q \cdot \mu \cdot l}{A_T \cdot \Delta P}, \quad (1)$$

where the terms are: k : permeability [m^2]; Q : flow rate [m^3/sec]; μ : dynamic viscosity [Pa sec]; l : length of the sample [m]; A_T : area perpendicular to the flow direction (see Fig. 2) [m^2], and ΔP the pore pressure drop over length l . [Pa].

The flow rate is calculated from:

$$Q = \frac{Ppdisp}{\Delta t} \cdot A_{pp} \quad (2)$$

where: $Ppdisp$ is given by pore-pressure intensifier displacement [m]; Δt : time interval [sec]; A_{pp} : cross-sectional area of pore-pressure intensifier piston [m^2].

Furthermore, the equivalent hydraulic aperture of the artificial fracture between the two sample plates, w , is evaluated as a function of the recorded flow rate, the sample width d , and the pressure drop measured over the sample length as (Fig. 2 shows details of the geometry):

$$Q = d \cdot \frac{w^3}{12 \cdot \mu} \cdot \frac{\Delta p}{dl} \quad (3)$$

Two identical suites of experiments were completed on samples of diorite and novaculite. Experiments were conducted at room temperature and with a pore fluid pressure gradient Δp of 0.1 MPa. Each experiment suite included three values of effective normal stress (5, 10, and 20 MPa) and shear displacements of 15 to 18 mm at a shear loading rate of 5 $\mu\text{m}/\text{sec}$, and confining pressures of 3 to 6 MPa (see Table 1 for other details).

<i># Test</i>	σ_n [MPa]	P_c [MPa]	P_p [MPa]	σ'_n [MPa]	<i>Rock</i>
P1083	20	6	0.1	19.9	Diorite
P1159	10	6	0.1	9.9	Diorite
P1082	10	6	0.1	9.9	Diorite
P1081	5	3	0.1	4.9	Diorite
P1168	20	6	0.1	19.9	Novaculite
P1080	20	6	0.1	19.9	Novaculite
P1114	10	6	0.1	9.9	Novaculite
P1101	5	3	0.1	4.9	Novaculite
P1079	5	3	0.1	4.9	Novaculite

Table 1. Experiment Variables.

The topography of the fracture surfaces was measured using the LLNL profilometer [35] before and after shear in the runs at effective normal stress of 20 MPa. Resolution is $\pm 5\mu\text{m}$ perpendicular to the fracture and we sampled at both coarse and fine resolution within the fracture plane. A lateral spacing of 0.1 mm covering an area of 4×4 mm (40×40 points) comprises the finely resolved profile, with the coarse profile comprising a grid of points spaced at 1mm over an area of 40×40 mm (40×40 points)

2.3 Results

2.3.1 Mechanical Behavior

The evolution of shear stress as a function of shear displacement is shown in Fig. 3. For both samples, shear stress shows an initial rise (before 8 mm) that scales with normal stress and culminates in a peak strength, followed by shear at a residual strength. In the case of diorite (at effective normal stress of 10 MPa) and novaculite (at effective normal stress of 10 and 20 MPa) a third peak is present at large offsets, interpreted as an experimental artifact. The peak shear stress (strength) ranges from 3 to 12 MPa for the diorite and 3 to 15 MPa for the novaculite. In both cases, peak stress and the following residual values are linearly proportional to the applied normal load as shown in Fig. 4. Data points in Fig. 4 indicate that

experimental reproducibility is quite good, with values of peak and residual strength within ± 1 MPa for a given normal stress.

Fig. 3. Shear stress as a function of loading shear displacement for diorite (a) and novaculite (b) at a range of effective normal stresses (see Table 1). Note definitions of peak and residual shear stress, which are shown in Fig. 4.

Fig. 4. Peak and residual shear stress values as a function of effective normal stress for diorite (a) and novaculite (b).

2.3.2 Hydraulic Behavior

The evolution of permeability as a function of fracture shear displacement is broadly consistent for diorite and novaculite (Fig. 5). Two isolated cases exist: one in diorite at an effective normal stress σ of 10 MPa (p1082) and one in novaculite at 20 MPa (p1080). These are outliers are attributed to technical problems in those experiments.

Fig. 5. Permeability as a function of shear displacement for diorite (a) and novaculite (b), at a range of effective normal stresses.

Initial permeability, prior to shear, ranges from 0.5 to $1 \times 10^{-14} \text{ m}^2$, independent of stress and rock type. With shear displacement, fracture permeability drops to a final value equal to $0.5 \times 10^{-17} \text{ m}^2$ recorded at effective normal stresses of 10 and 20 MPa, in diorite; while in novaculite, the final permeability is one order of magnitude higher: $0.5 \times 10^{-16} \text{ m}^2$ (at σ of 20 MPa).

We show the relationship between permeability, shear strength, and shear displacement for diorite in Fig. 6. These results indicate that at 5 MPa effective normal stresses (Fig. 6a) there is little change in permeability with shear. At an effective normal stresses of 10 MPa (Fig. 6b) and above (Fig. 6c) permeability drops sharply upon reaching the peak strength and then reaches a steady value with continued shear.

Fig. 6. Plots showing the relationship between permeability, shear stress, and shear displacement for diorite at effective normal stresses of (a) 5 MPa, (b) 10 MPa, and (c) 20 MPa.

2.3.3 Chemical Behavior

During each test the discharged pore fluid was collected for chemical analysis of the dissolved components; only the elements with the highest aqueous concentrations are reported in Fig. 7. Of the measured components, only magnesium concentrations are highest and are the only components to vary appreciably with the applied effective normal stress. However, Mg is a contaminant in the pore fluid from the testing equipment and is not considered further here. Aqueous concentrations of the other components increase slightly with shear displacement during the experiments on diorite (K) and show a larger increase with displacement for novaculite (Si).

Fig. 7. Concentration of major ions in the pore fluid as a function of net shear displacement for diorite (a) and novaculite (b) at a range of effective normal stresses (Table 1).

2.4 Discussion and Conclusions

Our experiments were designed to determine the evolution of strength and permeability of artificial, relatively-smooth fractures in diorite and novaculite. We find that shear stress evolves with shear displacement, with steady state values reached after ~10 mm (diorite) and ~15 mm (novaculite) of load point displacement. En route to the peak strength, multiple peaks in shear stress are observed in some cases. The first systematic peak usually occurs before 2 mm and is attributed to stretching of the sample-encasing rubber membrane. The remaining peaks are interpreted as functions of the asperity distribution of the contact surfaces.

Although all the samples were roughened in the same manner using 60# grit polishing compound, the resulting surfaces in novaculite appeared smoother than those in diorite (Figs. 8-10). The profiles for the samples are shown pre- and post-test (Figs. 8-10) and these show changes in the short wavelength

roughness as a result of shearing. The pre-test images of roughness show sharp peaks in the asperity distribution; and these are removed as a result of shearing. At coarser resolution, the post-test distributions for diorite show longer wavelength features of the roughness spectrum (Fig. 10).

Fig. 8. Surface roughness images determined from probe profilometer. Relative range (x , y , z) is the same for each image. (a) Pre-test surface of the large (45 x 70 mm) diorite block (see Fig. 2). (b) Pre-test surface of the smaller (45 x 50 mm) diorite block. (c) Post-test surface of the large (45 x 70 mm) diorite block; same surface as in (Fig.8a).

Fig. 9. Surface roughness images determined from probe profilometer. Relative range (x, y, z) is the same for each image. (a) Pre-test surface of the small (45 x 50 mm) novaculite block (see Fig. 2). (b) Post-test surface of the smaller (45 x 50 mm) novaculite block.

Fig. 10. Surface roughness images determined from probe profilometer. These are coarser (x, y) views of the images shown in Figure 9. (a) Post-test surface of the small (45 x 50 mm) diorite block. (b) Post-test view of the larger (45 x 70 mm) diorite block.

The images of surface roughness provide important information for understanding the evolution of friction with shear (Fig. 11). For diorite, the stress-displacement curves indicate that asperities are sufficiently smooth that fracture slip occurs without long-term slip hardening (Fig. 3). On the contrary, for novaculite, we see a prominent second peak strength between 10 and 15 mm of slip. This suggests that the asperity height distribution is broad, with few or no prominent features. Fig. 11 shows the coefficient of friction μ (ratio between shear and effective normal stresses) as a function of the shear displacement. For both rock types, the residual friction value ranges between 0.6-0.7 and this is justifiable considering the final evolution of the smooth surface in the samples. These data are consistent with expectations for friction between two flat plates, which is principally related to the roughness of the surfaces rather than their composition.

Fig. 11. Friction coefficient as a function of shear displacement for diorite (a) and novaculite (b) at each effective normal stress.

Results show that both in diorite and in novaculite the initial values of fracture permeability range between $0.5\text{-}1.0 \times 10^{-14} \text{ m}^2$, independent of the effective normal stresses. This equates to equivalent hydraulic apertures in the range 15-20 μm (see Fig. 12). Upon shearing the permeability drops to the final steady value of $0.5 \times 10^{-17} \text{ m}^2$ recorded at effective stresses of 10 and 20 MPa and corresponds to an

equivalent hydraulic aperture to 2 μm in diorite. Novaculite behaves similarly but the final permeability is $0.5 \times 10^{-16} \text{ m}^2$ and it is obtained only at an effective normal stress of 20 MPa.

Fig. 12. Hydraulic aperture determined from hydraulic conductivity, assuming the cubic law for fracture flow, as a function of shear displacement for diorite (a) and novaculite (b) at each effective normal stress.

The evolution of permeability during shear is clearly related to surface roughness and the development of wear products. Magnitudes of pre-shear permeability are only weakly related to the roughness of the contacting surfaces – evidenced since all surfaces return similar magnitudes of initial permeability, and these are insensitive to normal stress. Although the shear resistance is influenced by roughness, with multiple peaks in shear resistance ascribed to the characteristics of the roughness profile, this influence has little impact on post-peak permeabilities. This observation is consistent with the production of wear products during shear.

In the case of diorite, in which the initial surfaces are rougher than for the novaculite, the production of gouge occurs more readily. Significant gouge is produced, as evidenced by the permeability response, at earlier shear offsets (at 6 mm offset in diorite compared with at 17 mm in novaculite at 20 MPa), and at lower stresses (already at 10 MPa for diorite). The observation that the permeability in diorite is the same at effective stresses of either 10 or 20 MPa can be explained by considering that the wear rate is

approximately constant, independent of normal stress in this range. Finally, the difference in the large-offset permeabilities observed at all stresses in diorite and novaculite are attributed to the relatively larger production of wear products in the higher amplitude roughness of the diorite. As expected, where mean permeabilities are converted to equivalent hydraulic apertures (Fig. 12), the apertures mirror the consistency between permeabilities recovered in a single rock type but at multiple stresses, and emphasize the difference between rock types. Although reducing data to an equivalent hydraulic aperture is inappropriate where permeability is controlled by wear products, the evolution of pre-shear apertures from between 15 and 20 μm to final values of 2-4 μm (diorite) and 5 μm (novaculite) is consistent with a model implicating wear products.

Observed aqueous concentrations at outlet increase slightly with shear offset in the experiments, on diorite and increase more markedly for the experiments on novaculite. This increase is attributed to the corresponding anticipated generation of wear products. Except for the presence of magnesium (implicated as a residue in the fluid capture system from prior experiments), all components increase in concentration with both shear offset and the corresponding duration of the test (Fig. 7). These twin effects of shear offset and residence time can be separated by noting that multiple void volumes flush the sample in a single experiment. Thus the observed increase in concentration with time is linked most strongly to the evolution of increased surface area from the development of comminution products. These concentrations and related rates of dissolution are rapid in a geologic sense, and are sufficiently rapid to have influence in engineering timeframes.

These experiments are reported with rigorous control on stress and fluid transport conditions, but with relatively less control on the evolution of surface topography and the effects of wear. Regardless, the role of wear products in mediating changes in permeability with offset, is largely independent of initial conditions of surface roughness, and especially insensitive to magnitudes of normal stress level. Correspondingly, inferences in the evolution of permeability may be linked to initial magnitudes of surface roughness and in the corresponding potential to generate wear products, in part related to the granular or crystalline nature of the rock type.

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3 CHAPTER 3: NUMERICAL SIMULATION OF THERMAL-HYDROLOGIC-MECHANICAL-CHEMICAL PROCESSES IN DEFORMABLE, FRACTURED POROUS MEDIA

Abstract

A method is introduced to couple the thermal (T), hydrologic (H), and chemical precipitation/dissolution (C) capabilities of TOUGHREACT with the mechanical (M) framework of FLAC^{3D} to examine THMC processes in deformable, fractured porous media. The combined influence of stress-driven asperity dissolution, thermal-hydro-mechanical asperity compaction/dilation, and mineral precipitation/dissolution alter the permeability of fractures during thermal, hydraulic, and chemical stimulation. Fracture and matrix are mechanically linked through linear, dual-porosity poroelasticity. Stress-dissolution effects are driven by augmented effective stresses incrementally defined at steady state with feedbacks to the transport system as a mass source, and to the mechanical system as an equivalent chemical strain. Porosity, permeability, stiffness, and chemical composition may be spatially heterogeneous and evolve with local temperature, effective stress and chemical potential. Changes in total stress generate undrained fluid pressure increments which are passed from the mechanical analysis to the transport logic with a correction to enforce conservation of fluid mass. Analytical comparisons confirm the capability of the model to represent the rapid, undrained response of the fluid-mechanical system to mechanical loading. We then focus on a full thermal loading/unloading cycle of a constrained fractured mass and follow irreversible alteration in *in-situ* stress and permeability resulting from both mechanical and chemical effects. In a companion paper [1] we examine a prototypical enhanced geothermal system (EGS) for changes in mechanical and transport properties, and outline in greater detail the strength of coupling between THMC mechanisms.

3.1 Introduction

It is well known that fractured rocks exhibit changes in mechanical compliance and hydraulic conductivity when subjected to thermal, hydraulic, mechanical, and chemical forces. In many engineering applications it is important that we are able to predict the direction and magnitude of these changes. However, the interplay between temperature, effective stress, chemical potential, and fracture response is complex; not only influenced by anisotropic and spatially varying fracture properties, but also by fracture properties that are dynamic, and evolve with the dynamic nature of the applied forces.

The gaping or sealing of natural fractures has clear implications in reservoirs for the sequestration of CO₂ [2] and radioactive waste repositories [3], where the release of CO₂ or the redistribution of pore fluids around contained radioactive waste is a primary concern. Volcanic environments are also impacted, as in the case of failing volcanic domes [4], where elevated fluid pressures may destabilize an existing volcanic pile. In other cases, such as petroleum or gas reservoirs, hot dry rock [5] or enhanced geothermal systems [6] (HDR/EGS), engineered stimulations may beneficially improve fluid circulation; a topic of

significant interest since the majority of worldwide geothermal capacity is contained within low permeability rock masses [6,7].

Despite their importance, the competing influence of processes that degrade fluid conductivity in dominant fractures, such as thin-film pressure solution [8-10] and mineral precipitation, and those that enhance it, such as shear dilation [11,12], mineral dissolution[13-15], and strain energy driven free-face dissolution [9,16] has yet to be addressed at geologic scale. To examine these processes in unison, we require an uncommon link between chemical and mechanical behaviors that maintains dependence on thermal and hydrologic changes. This is THMC coupling. And while several THM [e.g. 3,17-20] and THC [e.g. 14] coupling methodologies have been suggested, to the authors' knowledge no single numerical simulator has been introduced to examine THMC processes in a construct that is applicable to the broad variety of above mentioned engineering applications.

Fig. 1 illustrates the potential error in excluding the chemical-mechanical link from numerical modeling. In the figure we follow a complete cycle of thermal/stress loading in a chemically active fractured rock. During the loading/unloading cycle, reversible (elastic) and irreversible (chemical-mechanical: pressure solution or other) changes in aperture occur, with the ultimate result that after unloading, once the system has been returned to its initial background state, we see an irreversible aperture reduction, and a corresponding irreversible loss in the state of stress. These two occurrences (7 and 8 in Fig. 1) are the behaviors of primary interest, as they indicate a complete and potentially significant alteration of the resting system that cannot be represented without the inclusion of THMC processes.

Fig. 1. Conceptual, behavioral trend of thermally loaded, fractured rock. A.) Follow light grey line as (1) increasing temperature builds stress (partially reduced by elastic fracture strain). (2) Irreversible fracture strains reduce stress, which, for illustrative purpose, is applied at the end of loading (3). Thermal unloading follows the black line. B.) Follow grey temperature (stress) loading line (4) elastic reduction in fracture aperture (idealized as linear). Loading reaches maximum value (5). Aperture irreversibly closes (chemical strain) and causes corresponding drop in stress. Black (6) unloading line returns the system to its resting state for an (7) irreversible aperture reduction and (8) corresponding irreversible stress loss.

3.2 Model Capabilities

In the following we introduce and implement a method for coupling the multiphase, multi-component, non-isothermal thermodynamics, reactive transport, and chemical precipitation/dissolution capabilities of TOUGHREACT [14] with the mechanical framework of FLAC^{3D} [21] to generate a coupled THMC simulator. This “modular” approach, first proposed by Settari [22] to couple geomechanics with reservoir

flow simulation, has some advantages over the development of a single coupled program. Modular approaches will typically be more rapid and less expensive to develop, although working within the framework of an existing code can sometimes lack the freedom that is inherent in “from scratch” code development. Additionally, as pointed out by Settari and Mourits [23], the modular construction allows for easier implementation of future advances in constitutive relationships or modeling structures (rather than modifying an entire coding structure), and the system can utilize highly sophisticated, rigorously validated existing codes developed at high cost. It can take many years for a new modeling structure to be validated by the research community, but in the case of TOUGHREACT and FLAC^{3D}, each has been extensively scrutinized and each code is “qualified” for regulated programs, such as the US radioactive waste program.

Furthermore, single codes often simplify behavior beyond the principal scope of the analysis. For example, complex geomechanical codes may represent the flow system as only single phase, and complex reactive transport codes often incorporate mechanical response as invariant total stresses. Appropriate coupling enables the important subtleties of geomechanical response to be followed while maintaining complex fluid thermodynamics and reactive processes. Although development time is shortened in this modular approach, execution times are commonly extended, as neither code is optimized for the couplings, and data transfer must occur between the concurrently or sequentially executing codes. As suggested by Settari and Mourits [23] and Minkoff et al. [24], however, this may not always be the case, because in systems where geomechanics may be loosely coupled (not changing at a rapid pace) the geomechanics simulation may not need to be conducted very often, thus improving computational efficiency over fully coupled codes where mechanics are equilibrated at every fluid flow time step.

The coupled analysis that we present incorporates features unique to engineered geosystems (particularly those under elevated temperature and chemical potential), involving the undrained pressure response in a dual-porosity medium and stress-chemistry effects including the role of mechanically mediated chemical dissolution of bridging fracture asperities. FLAC^{3D} is exercised purely in mechanical mode, where undrained fluid pressures may be evaluated (externally) from local total stresses. This undrained methodology allows calculation of the short-term build-up in fluid pressures that result from an instantaneous change in stress, provided we have knowledge of the compressibility of the pore fluids and the solid matrix. In this way, the complex thermodynamics of phase equilibria of multiphase water mixtures, and even multi-component mixtures (such as CO₂ and water), can be tracked in the pre-existing framework of TOUGHREACT. As TOUGHREACT has no use for compressibility, however, it is necessary to code this capability into the program or, as we have done, to insert a thermodynamic calculation into the external linking module (discussed later). For water mixtures, we utilize the 1997

International Association for the Properties of Water and Steam (IAPWS) steam table equations [25]. For CO₂ mixtures, an appropriate equation of state would be required, and we have not yet added this capability. If a system is unsaturated (such as in HDR/EGS), fluid compressibility is very large, and the undrained poroelastic equations approach their drained counterparts. Therefore, while our construct is tailored to saturated systems, drained systems are automatically accommodated.

FLAC^{3D} is applied independent of time to accommodate the incremental equilibration of stresses for various mechanical constitutive relationships. TOUGHREACT performs time-dependent transport calculations, tracking thermodynamic relationships for temperature, phase equilibria, and pore pressure dissipation together with aqueous chemical equilibrium and kinetic precipitation/dissolution in a dual-porosity medium. Under large thermal stresses, shear failure may be expected, and FLAC^{3D} is capable of handling this with the constitutive theories of Mohr-Coulomb or Hoek-Brown. Plastic flow is also possible, although this would require consideration of permeability changes that occur during fracture shear and also fracture compression. This complexity is not addressed here, and will be the topic of a future manuscript.

3.3 Simulation Logic

Simulation is executed within FLAC^{3D}'s FISH programming language [21], where external operations by TOUGHREACT and the linking module are controlled. TOUGHREACT, an integral finite difference code [26], calculates all properties at the central coordinate of element volumes. In contrast, the first order finite difference program FLAC^{3D}, with explicit temporal derivatives and a mixed discretization method that overlays constant strain-rate tetrahedral elements with the final zone elements (adding greater freedom in methods of plastic flow), utilizes properties of state (p , T) at corner nodes and mechanical variables (σ , u) at central coordinates. Correspondingly, state properties from central TOUGHREACT nodes are interpolated to connecting corner nodes of FLAC^{3D}. Stress (not displacement) outputs from FLAC^{3D} are used as the independent variable in constitutive relationships. The parsing of stresses to TOUGHREACT is direct, as they are calculated centrally within the node-centered blocks of FLAC^{3D} (in spatial agreement with TOUGHREACT).

In its current construction, the codes iterate upon the same numerical grid. This structure, however, is not required. As pointed out by Minkoff et al. [24], un-matched meshes are one benefit to a modular code. For example [24], it may be desirable to conduct flow simulations upon a reservoir area impacted by fluid injection and withdrawal only, while the mechanical grid may include the reservoir area in addition to all overburden up to the ground surface. Neither must the overlapping simulation areas utilize identical grid spacing, such that it may be desirable to refine the fluid flow mesh to capture some complex physics in a

specific area, without adapting the mechanical mesh to agree. It is only required that interpolation of data accommodate the differences in mesh extent and geometry.

Sequential execution of the two programs is linked by a separate code capable of parsing data outputs from each primary simulator as input to the companion. This separate code is referred to as the “interpolation module”. The module is a Fortran 90 executable, and maintains access to data outputs from TOUGHREACT and FLAC^{3D}. In addition to data interpolation, this module executes constitutive relationships including permeability evolution, dual-porosity poroelastic response to stress, and thermodynamically controlled fluid compressibility.

Fig. 2. Coupling relationship between TOUGHREACT, FLAC^{3D}, and the interpolation module.

All transient calculations take place within TOUGHREACT, and it is here that the time step is controlled for conditions of fluid velocity, grid size, and reaction rates. Additionally, there is a secondary (explicit) time step that controls how often stress is corrected to changes in fluid pressure (for what length of time TOUGHREACT conducts a flow simulation before allowing stress equilibration in FLAC^{3D}). This frequency is controlled in the interpolation module. If the magnitude of stress change in the system over one time step is beneath a pre-determined tolerance, the frequency is decreased (if stress is not changing, mechanical re-equilibration is unnecessary), and vice versa for an upper tolerance. Coupling is explicit and constitutive calculations are performed once per iteration (assuming constant constitutive values throughout a fluid flow time step), requiring sufficiently small time steps relative to the rapidity of change

in the system. The validity of utilizing such a methodology is discussed in later sections to provide insight into this explicit time step.

The coupling cycle is shown in Fig. 2, and is comparable to the loose coupling, modular structure of Minkoff et al. [24] and Rutqvist et al. [3]. Simulation begins with equilibration of temperature (T) and pore fluid pressure (p_f) in TOUGHREACT, where porosity (ϕ) change due to mineral precipitation/dissolution and liquid saturation (S) are also obtained. Constitutive relationships in the interpolation module transform these outputs into fluid bulk modulus (K_f), as obtained from IAPWS steam table equations, and permeability change due to mineral behavior (Δk_{TC}). The TOUGHREACT central node data (p_f , T) are then interpolated to corner node information as input to FLAC^{3D}. After stress equilibration in FLAC3D, the interpolation module uses stress outputs within a dual-porosity framework, consisting of matrix ($p_f^{(1)}$) and fracture ($p_f^{(2)}$) pore fluid pressures, to obtain the pressure response to the new stress field via domain (*matrix*, *fracture*) and state (p , T) specific Skempton coefficients. Effective stress is then used to obtain the permeability change due to pressure solution type behavior (Δk_{TMC}) while chemical strain (ϵ_C) is accommodated in the stress field (discussed later). Parameters then re-enter TOUGHREACT for the next time step.

3.4 Governing equations

The physical system of interest is modeled herein as a multi-continuum, fully or partially saturated fracture/matrix system with direct communication between the domains. Local thermal equilibrium is assumed between the fluid and solid (at a single point in continuum space, the fluid and solid exhibit the same temperature), but not between separate fracture and matrix domains. From this framework, a differential of pressure and temperature may develop between the fracture and matrix, with properties of pressure and temperature dissipation influencing the rapidity of transfer from local changes in the fracture system into the surrounding matrix blocks, and vice versa. As such, the multi-continuum distinction is fully maintained within the numerically represented THC system, while local continuity of stress requires equilibrium of stresses between fracture and matrix, which is then represented within the single continuum framework of FLAC^{3D}. For this transition, physical characteristics are delegated based upon dual-porosity poroelastic theory [27-31]. The governing balance equations and their constitutive counterparts are discussed below.

3.4.1 Conservation of momentum – solid

Mechanical equilibrium of the solid phase is governed by the balance of linear momentum,

$$\sigma_{ij,j} + b_i = \rho \dot{v}_i, \quad (1)$$

where b_i are the body forces per unit volume, $\dot{v}_i$ are the material time derivatives of velocities, and $\sigma_{ij,j}$ represents the divergence of the *Cauchy* stress tensor transpose. In an iterative formulation, for static equilibrium of the medium, acceleration approaches null, and the momentum balance becomes the common force equilibrium relation (*Cauchy* equation of equilibrium),

$$\sigma_{ij,j} = -b_i. \quad (2)$$

The resulting unknowns can be accommodated through any of several elastic or plastic closure relationships. In this work, we begin with the case of an isotropic, elastic solid, thus introducing the stress/strain constitutive relationship for a medium with two distinct porosities (see dual-porosity discussion below), including the effects of pore fluid pressure, p , and temperature, T (a combined equation utilizing constitutive poroelasticity [e.g. 32 eq. 7.42], with thermoelastic response, and utilizing two distinct pore fluid pressures as in Wilson and Aifantis [27]),

$$\sigma_{ij} = 2G\varepsilon_{ij} + \frac{2G\nu}{1-2\nu}\varepsilon_{kk}\delta_{ij} - (\alpha_p^{(1)}p + \alpha_p^{(2)}p)\delta_{ij} - \alpha_T T\delta_{ij}, \quad (3)$$

where G is shear modulus, ν is Poisson ratio, $\alpha_p^{(i)}$ and α_T are the coupling coefficients for fluid and thermal effects for the $^{(1)}$ fracture and $^{(2)}$ matrix, δ_{ij} is the *Kronecker* delta, and the linearized (“small”) strains may be defined in relation to the gradients of displacement as the symmetric part of $u_{i,j}$, or,

$$\varepsilon_{ij} = \frac{1}{2}(u_{i,j} + u_{j,i}). \quad (4)$$

Inserting Eq. (4) into Eq. (3) and the result into the equilibrium equation, Eq. (2), yields a *Navier*-equation defined in terms of incremental displacements (u),

$$G\nabla u_i + \frac{G}{1-2\nu}u_{k,ki} = (\alpha_p^{(1)}p_{,i} + \alpha_p^{(2)}p_{,i}) + \alpha_T T_{,i} - b_i, \quad (5)$$

which is the so-called displacement formulation of force equilibrium for an isotropic, elastic solid with distinct fracture and matrix pore fluid pressures.

3.4.2 Conservation of momentum, mass, and energy – fluid

Fluid, aqueous species, and energy are transported through the system as defined by their respective mass and energy balances. The master equation for these processes is given in integral form as,

$$\frac{d}{dt} \int_V M_\kappa dV = \int_\Gamma \mathbf{F}_\kappa \cdot \mathbf{n} + \int_V q_\kappa dV, \quad (6)$$

where the left-hand side represents the rate of accumulation of the conserved quantity (M_κ is mass of fluid, mineral mass, or energy density) resulting from the arrival of the fluxes $\mathbf{F}_\kappa$, (of fluid, mass, or energy) across the boundary, Γ , and complemented by volume sources, q_κ , distributed over the nominal element volume, V , for each component, κ (gas, liquid, advected species, or heat). In this discussion we

have adopted (for clarity of coefficients) standard tensor notation, where bold values represent first or second order tensors. Eq. (6) may be transformed into its common PDE counterpart through application of the divergence theorem (where the integral vanishes due to the arbitrary nature of the representative elementary volume),

$$\frac{\partial M_{\kappa}}{\partial t} = -\nabla \cdot \mathbf{F}_{\kappa} + q_{\kappa}, \quad (7)$$

where the mass, flux, and source terms *must then be independently determined* for a given system.

Mass, or energy density, M_{κ} , in Eq. (7) is defined for each component, κ , as the summation of the various contributions to the component across all phases (subscripted l, g, s for liquid, gas, or solid) as,

$$M_{\kappa} = \phi S_l \rho_l X_l + \phi S_g \rho_g X_g + (1 - \phi) \rho_s X_s, \quad (8)$$

where S is phase saturation, ρ is density (or species concentration), ϕ is porosity, and $X_{s,l,g}$ is mass fraction (or internal energy). Simplification then occurs for each calculation. The third term disappears for fluid mass calculations (no solid phase present), while the second and third terms are excluded from aqueous species mass (species may be present within the liquid medium, but not solid or gaseous).

Fluxes, $\mathbf{F}$, in Eq. (7) are given by the summation across phases ($\beta = l, g$) of the advective and diffusive terms as,

$$\mathbf{F} = \sum_{\beta=l,g} \left(-X_{\beta} \rho_{\beta} \frac{\mathbf{k} k'_{\beta}}{\mu_{\beta}} (\nabla p_{\beta} - \rho_{\beta} \mathbf{g}) \right) - \lambda_{\beta} \nabla C, \quad (9)$$

where the first term represents the contribution of advection through consideration of the multiphase extension of *Darcy's* law for relative permeability, k' , intrinsic permeability vector, $\mathbf{k}$, dynamic viscosity, μ , and, as before, ρ is density of fluid (or concentration of species) and X is mass fraction for fluid transport, specific enthalpy for heat flow, or unity for chemical calculations. The second term represents diffusive transport as governed by the laws of *Fick* and *Fourier*, and introduces conductivity, λ_{β} , and gradient (of temperature or concentration), ∇C . This last diffusive term is only present when calculating the flux of temperature or concentration, and therefore disappears when calculating pure liquid flux. For heat flow calculations, λ_{β} is thermal conductivity, while for chemical flux $\lambda_{\beta} = \rho_{\beta} \tau \theta S_{\beta} D_{\beta}$ with tortuosity, τ , and diffusion coefficient, D_{β} . Importantly, a hydrodynamic dispersion concept is not utilized in the classic *Fickian* sense. Instead, TOUGHREACT utilizes the interaction of regions with differing velocities (fracture and matrix in a dual-porosity construct) to induce solute mixing [see 33]. In the case of mineral mass, the flux term disappears (colloid transport is not considered).

The source term, q_{κ} , in Eq. (7) may be comprised of an injection or withdrawal source or as an increase in species concentration (or mineral mass) due to dissolution (or precipitation). A thermal source may also

arise due to a release of energy during chemical reactions. This last case is not currently considered. Sources of aqueous species and/or mineral mass are discussed in the following.

3.4.3 Chemical precipitation/dissolution

A generalized rate law for precipitation/dissolution of a mineral, m , is [34,35],

$$r_m = \text{sgn}\left(\log\left(Q_m / K_m^e\right)\right) k_m^c A_m f(a_i) \left| 1 - \left(\frac{Q_m}{K_m^e}\right)^\varphi \right|^n, \quad (10)$$

where k^c is the rate constant, A is the specific mineral reactive surface area per kg of H_2O , K^e is the mineral/water equilibrium constant, and Q is the ion activity product.. The function $f(a_i)$ represents some (inhibiting or catalyzing) dependence on the activities of individual ions in solution such as H^+ and OH^- [cf. 36], and $\text{sgn}(Q_m/K_m^e)$ provides a direction of reaction: positive for supersaturated precipitation. The exponential parameters, φ and n , indicate an experimental order of reaction, commonly assumed to be unity. An additional term (multiplied by Eq. (10)) may also be introduced to represent the dependency of reactive surface area on liquid saturation cf. 33]. Dependency of the rate constant may be handled, to a reasonable approximation [37], via the Arrhenius expression,

$$k^c = k_{25}^c \exp\left(-\frac{E_a}{R_u}\left(\frac{1}{T} - \frac{1}{298.15}\right)\right), \quad (11)$$

for the rate constant at 25°C, k_{25}^c , activation energy, E_a , and gas constant, R_u .

In the case of amorphous silica an alternate expression may be used following the work of Carroll et al. [38], where the precipitation rates reported in Rimstidt and Barnes [39] were observed to underestimate behavior in geothermal systems. This new rate law, based upon experimental data for more complex geothermal fluids, becomes, in a form modified by Xu et al. [40] to approach zero as Q/K approaches one (system approaches equilibrium),

$$r_m = \text{sgn}\left(\log\left(Q_m / K_m^e\right)\right) k_m^c A_m f(a_i) \left| \left(\frac{Q_m}{K_m^e}\right)^\mu - \left(\frac{K_m^e}{Q_m}\right)^{2\mu} \right|^n. \quad (12)$$

These are the formulations utilized in TOUGHREACT. Reactions between aqueous species (homogeneous reactions) are assumed to be at local equilibrium, and therefore governed by the relationship between the concentrations of basis (primary) species and their activities, partitioned by the stoichiometric coefficients. This relationship is termed the law of mass action [cf. 34]. The assumption of local equilibrium greatly reduces the number of chemical unknowns and ODE's (between primary and secondary species), and is accurate to the extent that the true reaction rates outpace the rate of fluid transport in a given system. This is a correct assumption for most aqueous species [34] (and flow

systems), but less so for slower redox reactions [33,34]. In TOUGHREACT, species activities are obtained from an extended *Debye-Hückel* equation with parameters from Helgeson et al. [41].

3.5 Deformable dual-porosity material

To represent the pressure loading of a fully or nearly liquid saturated system (particularly at high temperature and pressure and with multi-component liquids) coupling of the above formulation requires the undrained (instantaneous) response of pore fluid pressure to mechanical loading in both the fracture and matrix domains. Hydrologic considerations allow a timed pressure-dissipation response throughout the fracture dominated fluid system and between the fracture/matrix companionship following undrained loading.

Classically, a dual-porosity material is represented as a porous matrix partitioned into blocks by a mutually orthogonal fracture network [42,43]. In this scenario, permeability is much higher within the fracture network, thus allowing global flow to occur primarily through the fractures, while the vast majority of storage occurs within the higher porosity matrix (due to its larger global fraction of the medium). Interchange of fluid and heat between fractures and matrix, so-called “interporosity flow”, is driven by pressure or temperature gradients between the two domains.

Expansion of this classic two-domain interaction into “multiple interacting continua” [44,45] allows the gradual evolution of gradients between fracture and matrix through the existence of one or more intermediate continua placed, mathematically, some linear distance from the fracture domain. This development has allowed for numerical approximations to more accurately represent the slow invasion of locally (to the fracture) altered pressures and temperatures deeply into the matrix blocks, and introduced dispersive mixing that arises at the interface of zones with differing fluid velocities. While this multi-continuum methodology may be adopted in TOUGHREACT to represent dual-permeability fluid transport with uniformly constant stress fields in time, we do not seek such an expansion with respect to a flow-deformation response [see 46]. As such, a dual-porosity framework with two interacting continua (fracture and matrix) is utilized in this study, while a compatible poroelastic theory carries this behavior into the mechanical domain.

3.5.1 Fluid pressure response

Extension of Biot’s poroelastic theory [47-50] to a dual-porosity framework has been previously addressed [27-31,46,51]. The methodologies presented in these works provide an adequate framework for the phenomenological representation of poroelastic coefficients capable of describing flow-deformation response in such a medium.

Continuity of fluid mass is represented in a compressible media as,

$$\frac{\partial \zeta}{\partial t} + \nabla \cdot \mathbf{F} = 0, \quad (13)$$

where ζ is the increment of fluid content as in Biot and Willis [52], and comprises the relative motion between fluid and solid. Inserting Darcy's law for the flux term yields,

$$\frac{\partial \zeta}{\partial t} - \frac{k}{\mu} \nabla^2 p = q \quad (14)$$

Biot's [48] linear-poroelastic constitutive equivalence, for volumetric strain, e , is,

$$\begin{pmatrix} e \\ \zeta \end{pmatrix} = \begin{pmatrix} \frac{1}{K} & \frac{1}{H} \\ \frac{1}{H} & \frac{1}{R} \end{pmatrix} \begin{pmatrix} \sigma \\ p \end{pmatrix}, \quad (15)$$

where the coefficients $1/K$, $1/H$, and $1/R$ hold their original meanings as bulk drained compressibility, poroelastic expansion, and specific storage, respectively. Substituting,

$$B \equiv - \left. \frac{\delta p}{\delta \sigma} \right|_{\zeta=0} = \frac{R}{H}, \quad (16)$$

for the *Skempton* coefficient, $\alpha \equiv K/H$, for the *Biot-Willis* coefficient and,

$$\frac{1}{R} \equiv \left. \frac{\delta \zeta}{\delta p} \right|_{\sigma=0} = \frac{\alpha}{KB}, \quad (17)$$

for the specific storage, condensing Eq. (15) to relate fluid content to strain, and substituting its time derivative into Eq. (14) establishes the flow condition for a single-porosity medium with no fluid sources,

$$\frac{\alpha}{BK_u} \dot{p} + \alpha \dot{e} = \frac{k}{\mu} \nabla^2 p, \quad (18)$$

where we have utilized the relationship for undrained bulk modulus,

$$K_u \equiv \left. \frac{\delta \sigma}{\delta e} \right|_{\zeta=0} = \frac{K}{1 - \alpha B}. \quad (19)$$

Extending to a dual-porosity medium, we follow the same procedure leading to the dual-porosity form of Eq. (5), where Eq. (18) is modified to exhibit two separate fluid pressures (for fracture and matrix) with flow between them governed by, in its simplest form, an instantaneous pressure differential, $\Delta p = (p_1 - p_2)$ [42], to obtain two continuity relationships [28],

$$\frac{k^{(i)}}{\mu} \nabla^2 p^{(i)} = \frac{\alpha^{(i)}}{K_u^{(i)} B^{(i)}} \dot{p}^{(i)} + \alpha^{(i)} \dot{e} + (-1)^i \gamma \Delta p, \quad (20)$$

where i is not a repetitive index, but represents the existence of two separate equations for the matrix ($i = 1$) and fracture ($i = 2$), and γ is the cross coupling coefficient for flow exchange between the two domains

[cf. 53]. Equation (20) merely states that the divergence of fluid flux for a given control volume must equal the rate of accumulation within that volume, and is thus a statement of mass conservation.

3.5.2 Dual-porosity load response

The general linear relation between strain, increment of fluid content, total stress (σ), and pore fluid pressure (p), simply extends Eq. (15) to allow, again, for two separate fluid pressures [31],

$$\begin{pmatrix} \delta e \\ -\delta\zeta^{(1)} \\ -\delta\zeta^{(2)} \end{pmatrix} = \begin{pmatrix} c_{11}c_{12}c_{13} \\ c_{21}c_{22}c_{23} \\ c_{31}c_{32}c_{33} \end{pmatrix} \begin{pmatrix} -\delta\sigma \\ -\delta p^{(1)} \\ -\delta p^{(2)} \end{pmatrix}, \quad (21)$$

where the superscripts refer to the (1) matrix and (2) fracture domains. The single porosity coefficients of Biot are no longer applicable, and are replaced by the unknown coupling coefficients, c_{ij} , that may be designated via a phenomenological deconstruction similar to that of Biot and Willis [52]. The coefficient matrix can be shown symmetric [cf. 31] by the *Betti* reciprocal theorem. Performing manipulations of the above equation through isolation of independent components (i.e. long-time versus short-time limits) allows determination of the central coefficients (see detailed procedure in Berryman and Wang [31] and Elsworth and Bai [30]).

Herein we assume that $c_{23} = c_{32} = 0$ [see 31], which differs slightly from the procedure of Elsworth and Bai [30], Khaled et al. [28], and Wilson and Aifantis [27]. Examination of Eq. (21) shows that this assumption implies the following: an undrained application of stress that influences a change in fluid content for the fracture domain does so through modification of fracture fluid pressure, and does not influence that of the matrix. The reverse is also true, with the overall implication being, see discussion in Berryman and Wang [31], that in the undrained limit the matrix and fracture domains are completely separate. This can be considered a justification for a dual-porosity approach [31].

In our analysis, the purpose of dual-porosity elasticity is to attain *Skempton* coefficients representing both the fracture and matrix domains,

$$\begin{aligned} \delta p^{(1)} &= B^{(1)} \delta\sigma = -\frac{c_{12}}{c_{22}} \delta\sigma \\ \delta p^{(2)} &= B^{(2)} \delta\sigma = -\frac{c_{13}}{c_{33}} \delta\sigma \end{aligned}, \quad (22)$$

which represent the undrained ($\delta\zeta = 0$) build in pore fluid pressure in each domain for a given change in stress as provided by FLAC^{3D}. Relationships to calculate these two *Skempton* coefficients are provided in Table 2 of Berryman and Wang [31]. For this procedure, we choose as the known coefficients $K^{(l)}$, K , $K_s^{(l)}$, and K_s , where K_s is the solid grain modulus (in a microhomogeneous medium [cf. 54]) and the fluid bulk modulus,

$$\frac{1}{K_f} \equiv \frac{1}{V} \frac{\delta V}{\delta p} \bigg|_T, \quad (23)$$

is calculated in the interpolation module as a function of position, temperature, and pressure utilizing the IAPWS steam table equations [25]. For a complete reconstruction of the individual relations required to represent the dual-porosity poroelastic response, refer to Berryman and Wang [31] and addendums in Berryman and Pride [51].

3.5.3 Effect on the global mass balance

Injection of fluid mass into TOUGHREACT in the form of fluid pressure violates conservation of mass by an amount proportional to the compressibility of the local fluids. A change in pressure by this procedure necessitates a change in local fluid volume, and therefore appearing or disappearing mass. However, when the local element is fully saturated, a stiff fluid will not significantly respond (volumetrically) to stress induced pressure changes, while for unsaturated media even a

Fig. 3. Relationship between coupling methodologies. Interior looping may occur over n steps (at fixed time, $t = t^k$) to equilibrate the response of stress to an undrained increase in pressure. Alternatively, this inter-looping may be excluded in favor of a “leapfrog” method, where a single stress equilibration (run of FLAC^{3D}) is conducted per time step.

significant volumetric response will not in general dictate a noticeable change in mass. Nonetheless, we err on the side of safety and correct for this discrepancy with a recast of Eq. (23),

$$dV = \frac{1}{K_f} V dp \bigg|_T, \quad (24)$$

which indicates the volume (or mass) error due to an increase in pressure, dp (at a given temperature). To correct for potential mass loss, we alter elemental volumes (physically reduce the volume of the mesh element) within TOUGHREACT by this amount (in an integral finite difference formulation, this does not require the alteration of geometric coordinates). In our simulations, including both single and

multiphase flow with water/steam phase changes occurring, we have not detected total system mass losses greater than $\sim 0.01\%$ of total system mass.

3.6 Undrained fluid/mechanical response

We now examine the error that our formulation introduces to the fluid-mechanical coupling. Excluding constitutive approximations, error may be introduced into the coupling procedure as it has been described up to this point in two primary ways: 1.) explicit time step size, and 2.) the equilibration step between a stress change and its undrained pressure response (Fig. 3).

The first is a direct byproduct of explicit coupling, insomuch as an increase in time step (length of the TOUGHREACT fluid step between each mechanical equilibration), allows a greater amount of fluid pressure to diffuse between each mechanical equilibration, introducing error proportional to the fluid diffusivity and inversely proportional to the rate of mechanical change (not the amount of mechanical change per timestep, $d\sigma$, which implies proportionality to error, but the rate of change per unit time ($d\sigma/dt$), implying inverse proportionality).

The second form of error, shown in Fig. 3, is due to the nature of the undrained pressure response, which may not be fully accommodated by a single stress equilibrium step. In other words, at a given time step a fixed pressure field enters FLAC^{3D} and is accommodated by a calculated stress distribution. This stress distribution induces a modification of the previously fixed pressure field, and this new pressure field may, in turn, produce a redistribution of the stress field whether or not any fluid is allowed to diffuse (within TOUGHREACT). A number of steps may be required to find the true equilibrium magnitude of stress and pressure, which tends to asymptote at a value higher than is suggested by a single equilibration step. This is not necessarily a *Mandel-Cryer* type effect [55,56], which is a real occurrence and would require the action of a diffusing fluid pressure and redistribution of stresses around the diffusing magnitudes (although the behavior is comparable). The case where FLAC^{3D} is run once per explicit time step (single equilibration step) is referred to herein as the “leapfrog method” (see Fig. 3). Each of these possible error sources (¹explicit time step and ²*leapfrog* versus $p \rightleftharpoons \sigma$ iteration) requires further examination, which consequently leads to validation of the undrained fluid-mechanical coupling.

3.6.1 Fluid-mechanical couple: instantaneous loading

In one dimension, we may examine the accuracy of the fluid mechanical coupling in comparison to the classical fluid diffusion equation of hydrogeology [e.g. 57],

$$\frac{\partial p}{\partial t} - c_f \frac{\partial^2 p}{\partial z^2} = 0, \quad (25)$$

which is a specific poroelastic result of Eqs. (14) and (15) restricted to a one-dimensional column of soil (or rock) under constant applied vertical stress [cf. 58], and gives its form to the analytical solution for heat flow [59],

$$p(z, t) = \frac{4p_0}{\pi} \sum_{m=0}^{\infty} \frac{1}{2m+1} \exp(-\Psi^2 c_f t) \sin(\Psi z), \quad (26)$$

where $\Psi = (2m+1)\pi/2L$, and $p_0 = B^{(v)}\sigma_0$ is the initial undrained pressure response to the applied vertical stress (σ_0). The one-dimensional *Skempton* coefficient (*loading efficiency* in Wang [58]) is given by,

$$B^{(v)} = -\frac{B(1+\nu_u)}{3(1-\nu_u)}, \quad (27)$$

for the *Skempton* coefficient, B , and undrained *Poisson* ratio, ν_u . This is the canonical consolidation problem of a one-dimensional column of soil subjected to a constant vertical stress applied at $t = 0^+$ to the top of the column, with fluid pressure allowed to drain freely from the point of applied stress. A similar solution is available for column displacement u [e.g. 48,58],

$$\frac{\partial^2 u}{\partial z^2} = c_m \frac{\partial p}{\partial z}, \quad (28)$$

for *Geertsma's* [60] uniaxial expansion coefficient (consolidation coefficient), $c_m \equiv \alpha/K^{(v)}$, with uniaxial bulk modulus, $K^{(v)} = K + 4/3G$. Under the same boundary conditions as above, the analytical solution is [58],

$$\Delta u(z, t) = c_m p_0 \left[(L-z) - \frac{8L}{\pi^2} \sum_{m=0}^{\infty} \frac{1}{(2m+1)^2} \times \exp(-\Psi^2 c_f t) \cos(\Psi z) \right] \quad (29)$$

with definitions the same as for Eq. (26), and the instantaneous displacement at the time of stress application $u(z, 0^+) = \sigma_0(L-z)/K_u^{(v)}$, for the undrained uniaxial bulk modulus,

$$K_u^{(v)} = \frac{K_u(1+\nu_u)}{3(1-\nu_u)}. \quad (30)$$

All undrained parameters approach their drained counterparts as fluid compressibility becomes large, or fluid saturation approaches zero.

Results of a TOUGHREACT-FLAC^{3D} simulation mimicking these boundary conditions are presented against these analytical solutions in Fig. 4. A column of porous rock ($E = 13GPa$, $\nu = 0.22$) with displacements constrained laterally and pore pressure initially zero, is subjected to an applied vertical load, $\sigma_0 = 50MPa$, at $t = 0^+$, and pressure is allowed to drain freely from the top of the column only. Time step was chosen large enough to illustrate the error incorporated in very early times (near the time of undrained loading) due to the *leapfrog* method of simulation (see Fig. 3).

Fig. 4. Comparison of TOUGHREACT-FLAC^{3D} fluid-mechanical coupling simulation versus analytical results in 1-dimension. A.) Normalized ($p_0 = p(z,0) = B^{(v)}\sigma_0$) pressure diffusion response versus diffusive time ($t_D = ct/L^2$). B.) Normalized ($u_\infty = u(0,\infty) = \sigma_0 L/K^{(v)}$) displacement response versus diffusive time.

Pressure builds (and elastic displacement decreases) in the early stages as the model cycles between stress equilibration and undrained pressure response (*leapfrog* artifact). Following the instantaneous loading period (50MPa applied over one time step) numerical results overlay nearly identically the analytical solution as pressure diffuses and stress accommodates the pressure reduction. A slightly greater error occurs at points nearest the free draining surface (left-most curve in Fig. 4A) due to the explicit time step size, where a greater rate of fluid diffusion allows the fluid to move greater distances before being accommodated by a mechanical response.

3.6.2 Fluid-mechanical couple: constant loading rate

In light of Fig. 4, it is of interest to examine more precisely the error that arises while the sample is being loaded. To do so, we wish to utilize the same geometry, but apply the load gradually over a finite loading period at a given loading rate, $d\sigma_0/dt$ (rate of increase of applied load at the top of the column per unit time). Here, we maintain the one-dimensional form, but alter the governing diffusion equation (25) to accommodate a constant loading rate [cf 58],

$$\frac{1}{c_f} \frac{\partial p}{\partial t} - \frac{\partial^2 p}{\partial z^2} = \frac{c_m \mu}{k} \frac{d\sigma_0}{dt}, \quad (31)$$

with the series solution adjusted so that, as above, the free draining boundary is at $z = 0$ [59],

$$p(z, t) = \frac{c_m d\sigma_0}{dt} \frac{L^2 \mu}{2k} \left(1 - \frac{(L-z)^2}{L^2} - \frac{32}{\pi^3} \sum_{m=0}^{\infty} \frac{(-1)^m}{(2m+1)^3} \right. \\ \left. \times \exp(-\Psi^2 c_f t) \cos(\Psi(L-z)) \right) \quad (32)$$

Results of the gradual loading analysis are presented in Fig. 5. Loading rate refers to the rate of increase of applied load at the top of the column per unit time. The amount of load change per iteration ($d\sigma_0$) is a function of the time step (dt), so that a smaller load change is experienced per iteration as the time step is decreased. Time steps were chosen for A and B such that $d\sigma_0 = d\sigma_0/dt \times dt$ is the same magnitude in each case. From the figure, two primary conclusions are apparent: 1.) At the slowest loading rate (Fig. 5A) and smallest time step (and correspondingly smallest $d\sigma_0 = d\sigma_0/dt \times dt$) there is no difference between the *leapfrog* approach and a simulation with additional $p \rightleftharpoons \sigma$ iteration (*inter-looping*), proving the intuitive result that small explicit time steps absolve the need for *inter-looping*. In this case, if the time step is too large to capture the fluid-mechanical coupling then *inter-looping* has little effect because more error is introduced by the fluid mechanical couple than by the *leapfrog* method (evidenced by the fact that the dashed lines do not improve in accuracy over their corresponding solid lines). 2.) A faster loading rate (Fig. 5B) results in greater error due to the *leapfrog* method, but lesser error due to the explicit time step size (evidenced by the relative accuracy of all three dashed lines). In other words, mechanical change (loading) is faster relative to fluid diffusion, and so the explicit time step size may be larger and still accommodate the fluid-mechanical coupling because less frequent mechanical equilibration is required to keep up with the relatively slower fluid diffusion. However, precisely because the loading rate is faster, greater error will result due to the non-iterative equilibration of stress and pressure. Therefore, a larger time step is viable, but only with *inter-looping*. In any case, the system may be accurately represented with the proper selection of time step and iterative method for a given rate of mechanical change, and at the slower loading rate (likely closer to those that might be seen in natural systems) the *leapfrog* method

is sufficient provided that the explicit time step is reasonably small. For now, experimentation is required to guarantee an accurate coupling.

Fig. 5. Error (compared to analytical solution) in undrained pore pressure response for constant loading rate of one-dimensional vertical column for A.) slower loading rate ($d\sigma_0/dt = 5.0 \times 10^4$) and B.) faster loading rate ($d\sigma_0/dt = 5.0 \times 10^5$). “Leapfrog” method of simulation is solid gray line with data points. Additional inter-looping method is dashed black line.

3.7 THMC mediated aperture/permeability change

Having now examined the fluid-mechanical mechanism, we proceed to introduce further complexities that surround chemical behaviors. And, because constitutive behavior in a geological system is generally non-linear, responses mediated by stress, fluid pressure, temperature, and chemical potential often require empirical examination. Notably, permeability of the system may change by orders of magnitude in

response to changes in effective stress. In the following, we describe changes in permeability, resulting from both stress and chemical effects, utilizing the empirical relationship of Min et al. [61]. That relationship is further developed herein to accommodate unloading of fracture asperities in a manner that suggests fracture gaping may occur only through mechanical means (or by thermal contribution to the stress field). Section 7.1 presents the governing loading equations as found in Min et al. [61], while Section 7.2 illustrates a similar unloading construct to Min et al. [61], but unloading is allowed to occur only through mechanical means.

3.7.1 Loading behavior

Hydraulic aperture of a fracture under an applied effective stress, σ' , may be defined empirically as [3],

$$b_m = b_m^r + (b^0 - b_m^r) \exp(-\omega \sigma'), \quad (33)$$

where b_m is the hydraulic aperture (subscripted m indicating changes due solely to mechanical effects), b^0 is the aperture under no mechanical stress, b_m^r is the residual aperture at maximum mechanical loading and ω is a constant that defines the non-linear stiffness of the fracture.

The dissolution of bridging asperities may also reduce the effective aperture of the fracture. These “chemical” effects may be accommodated in the relationship for fracture aperture in a form that includes the mechanical compaction process of Eq. (33) and pressure solution –type dissolution of contacting asperities, where we have substituted $b_m^{\max} = b^0 - b_m^r$ as the maximum possible mechanical closure [61],

$$b_{mc} = b_m^r + \{b_m^r - b_c^r + b_m^{\max} \exp(-\omega \sigma')\} \cdot \exp(-\sigma'(\beta - \chi/T)) \quad (34)$$

where T is temperature and the empirical constants β and χ define the chemical compaction process. The subscripted c represents changes due to chemical effects and b_c^r is the residual aperture at maximum chemical loading. Buried within these two constants [see 61] is the critical stress [61 modified from 62,63],

$$\sigma_c = \frac{E_m (1 - T/T_m)}{4V_m}, \quad (35)$$

where E_m is the heat of fusion, T_m is the temperature of fusion, and V_m is the molar volume of the mineral comprising the fracture asperity. Dissolution of the contacting asperity will progress where the local asperity stress exceeds this critical stress that represents both the chemical and mechanical potential of the contact.

Permeability is evaluated for an orthogonal set of persistent fractures of spacing s , from the cubic law, [64,65] $k = b^3/12s$. Importantly, Eq. (34) represents equilibrium behavior, where chemically mediated changes have run to completion (it is a thermodynamic, not kinetic relationship).

3.7.2 Unloading behavior

The above constitutive relationship governs aperture closure under conditions of thermal/mechanical loading due to the effects of mechanical deformation (Eq. (33)) and chemical alteration including mechanical deformation (Eq. (34)). If utilized in its entirety and without memory of any previous mechanical/thermal state, this represents the case of complete reversibility. However, aperture closure should not be viewed as completely reversible or irreversible, but as a mechanism that is dependent on the initial stress state and subsequent loading, as well as one that maintains memory of some attained stress magnitude and a subsequent unloading period.

For instance, subsurface storage of radioactive waste is characterized by a loading period, during which temperature steadily increases and fracture apertures correspondingly decrease, followed by a period of sustained cooling towards the background state, implying a reversal of this process (fracture gaping). Alternatively, geothermal reservoirs are largely characterized by unloading behavior, where the maximum stress/temperature condition is the *in-situ* state of the fractured mass, and the injection of cooler circulation fluids causes unloading from this *in-situ* state. It is of some interest to determine the precise behavior of such an unloading period and its beginning transition.

The mechanical component of fracture closure is not a completely reversible process, but exhibits hysteresis as governed by both the elastic and plastic properties of the contacting asperities. Furthermore, while chemical behaviors may contribute to permeability *increase* through the action of thermodynamically governed dissolution, pressure solution type mechanisms as discussed above are incapable of inducing gaping of the fracture during an unloading stage (barring the inclusion of “force of crystallization” processes, pressure solution is irreversible). Therefore, it is apparent that an additional term is needed to describe the reversible *portion* of mechanical closure, while *excluding* the possibility of chemical reversibility. In this aim, we follow a procedure similar to that of Min et al. [61] to develop an unloading relationship, but maintain a reversibility that is due purely to mechanical effects.

Table 1. Parameters of the permeability constitutive relationship	
Parameter	Fitted
Residual mechanical aperture, b_m^r (μm)	6.0
Residual chemical aperture, b_c^r (μm)	3.0
Constant in aperture relationship, β	1.00
Constant in aperture relationship, χ	345
Stiffness coefficient, ($1/\text{MPa}$)	0.375
Mechanical recovery ratio, R_m	0.8

In the simplest formulation, this need may be addressed through a mechanical recovery ratio, R_m , that governs the degree of elastic reversibility, and is defined as the ratio of the potential *unloading* mechanical aperture change, $b_{m(u)}^{\max}$, to the maximum potential *loading* mechanical aperture change, $b_m^{\max}$, as,

$$R_m = \frac{b_{m(u)}^{\max}}{b_m^{\max}}. \quad (36)$$

It is first necessary to examine the case of a mass unloaded from a state of infinite stress with the unloading version of Eq. (33),

$$b_{m(u)} = b_m^r + b_{m(u)}^{\max} \exp(-\omega\sigma'), \quad (37)$$

or, from the definition of recovery ratio,

$$b_{m(u)} = b_m^r + R_m b_m^{\max} \exp(-\omega\sigma'). \quad (38)$$

However, the unloading process is dependent on the maximum loading stress (initial unloading stress). The difference in aperture between this maximum loading stress and some unloaded state is (utilizing Eq. (38)),

$$\Delta b_{m(u)} = R_m b_m^{\max} \exp(-\omega\sigma'_{(u)}) - R_m b_m^{\max} \exp(-\omega\sigma'_{\max}), \quad (39)$$

with the maximum (prior to unloading) effective stress $\sigma'_{\max} > \sigma'_{(u)}$, for any subsequent unloading effective stress, $\sigma'_{(u)}$. This inequality states that load cycling is not considered. The unloaded aperture is then comprised of the difference between this change and the fully loaded aperture, b^f ,

$$b_{m(u)} = b^f + \Delta b_{m(u)}. \quad (40)$$

In the case of mechanical loading and unloading, the aperture at maximum loading stress, b^f , is equivalent to the final loaded aperture, $b_m(\sigma'_{\max})$, and so the unloading aperture is obtained by substituting Eq. (33) into Eq. (40). However, we are seeking the relationship for a fracture that has been chemically and mechanically loaded, and then unloaded along a path defined by the recoverable portion of mechanical loading. Therefore, substituting $b^f = b_{mc}(\sigma'_{\max})$ and inserting Eq. (39) into Eq. (40) and simplifying yields,

Fig. 6. Comparison of the analytical results of Eqs. (34) and (41) against experimental results of Hardin et al. [66]. Experimental results are shown as black dashed line with solid data points. Gray solid line with hollow data points is the analytical solution. Each data point is numbered to correspond with the original data points of Hardin et al.

$$b_{m(u)} = b_{mc}(\sigma'_{max}) + R_m b_m^{\max} \left\{ \exp(-\omega \sigma'_{(u)}) - \exp(-\omega \sigma'_{max}) \right\}, \quad (41)$$

Where $b_{mc}(\sigma'_{max})$ is Eq. (34) evaluated at $\sigma' = \sigma'_{max}$. This relationship defines the aperture at a stress magnitude lower than and obtained *a posteriori* the fully loaded state. Equations (34) and (41) then fully define the loading and unloading cycle, respectively, of a fractured mass. The required empirical parameters are shown in Table 1. Parameters were obtained through a comparison with experimental results introduced in the heated block test of Terra Tek [66], where aperture was monitored during a complete loading and unloading cycle *in-situ*, on a 2x2 m cube of granitic gneiss subjected to stresses supplied by flatjacks with temperature alteration via borehole heaters. The original experimental results of Hardin et al. [66] are shown in Fig. 6 alongside theoretical reproduction of this behavior calculated with Eqs. (34) and (41). In the figure, loading begins at point 9 (and is isothermal for the first 3 data points) and continues until point 16 (non-isothermally), before being unloaded to the initial state at point 21. Hardin et al. also performed two intermediate load/unload cycles at points 13 and 16. These two intermediate cycles are not considered here, and the analytical solution is incapable of representing them. Agreement between the two data sets is satisfactory for the primary points of interest (intermediate

loading/unloading cycling is not considered), excluding point 19, where unloading aperture cannot be reproduced with the given analytical model (which is purely mechanical and does not undergo unloading with decreasing temperature unless the stress field is altered).

3.7.3 “Force of Crystallization”

Chemical precipitation is commonly assumed to cause a reduction in fracture aperture due to a buildup of deposited species along the fracture face. Contrary to this assumption is the concept of “force of crystallization”, dating back to 1896 with the work of Dunn [67] and 1920 with Tabor [68], with a phenomenological model presented by Weyl [8]. Force of crystallization operates analogously and inversely to pressure solution where, instead of relieving fracture stress through dissolution at asperity contacts, if the fluid is sufficiently super saturated mineral precipitation and crystal growth may exert pressure at contact points and lead to physical gaping of the fracture. Further discussion of the mechanism is available in the literature (e.g. [69-71]). While we do not, in a fundamental sense, implicitly consider the impact of this process in our model, the current logic is capable of accommodating this effect in a straightforward manner – should solution concentrations be sufficiently super saturated. The phenomenological relationship for pressure solution that we utilize is able to adequately match the laboratory studies on which it is based, all of which involve significantly under saturated fluids only.

3.8 THC mediated porosity/permeability change

Thermo-chemical induced changes in permeability may be referenced to precipitation/dissolution behaviors along the continuum fracture and matrix domains. Here, aperture changes are caused by the addition or removal of mineral components from the walls of (at the scale of these investigations) an assumed uniform fracture face, or an isotropic porous volume fraction. This is not precisely “free face dissolution” (which implies contribution of strain energy to thermodynamic dissolution), but a purely chemically driven process governed by the rates of reaction as previously discussed. In the following, we assume that processes of this type may act independently from pressure solution over a single time step, thus enabling them to be additive over that time step. This does not indicate process independence, which would allow chemical analyses to be conducted separately of TM or of TMC without loss of accuracy. These processes are still strongly dependent on one another outside of a time step. For example, changes in permeability from pressure solution (or chemical precipitation/dissolution) will alter the flow characteristics and residence times of circulating fluids, thus modifying thermal transport. Changes in local temperature in this manner alter the stress field and modify chemical reaction rates. Modified reaction rates and residence times influence the characteristics of chemical reaction, while modified temperature and stress influence pressure solution and thermal gaping.

Changes in fracture aperture due to THC behavior are accommodated via the chemical precipitation behavior incorporated in TOUGHREACT. Addition or removal of mineral mass from the continuum system results in a change in fracture or matrix porosity within a nominal element volume, as given by the overall change in the volume of minerals present by [40,72],

$$\phi = 1 - \sum_{m=1}^N f_m^{rx} - f^u, \quad (42)$$

Where f^{rx} is the volume fraction of mineral m in the surrounding rock $v_{mineral}/v_{medium}$ and f^u is the volume fraction of the non-reactive surrounding rock. Relations between fracture porosity and permeability are provided in the literature. One such possibility is a simple cubic relationship [34],

$$k = k_i \left(\frac{\phi}{\phi_i} \right)^3, \quad (43)$$

where the subscript, i , refers to an initial property and k , and ϕ are permeability and porosity, respectively. While several such relations may be implemented from within TOUGHREACT, it is necessary in our case to calculate permeability changes externally in order to operate multiple mechanisms simultaneously. Compatibility between the permeability change due to this behavior and that of pressure solution can be indexed to the change in fracture aperture by, as before, $b = \sqrt[3]{12ks}$. Aperture change via this mechanism is then assumed additive to the THMC aperture reductions associated with pressure solution driven compaction.

Several options also exist for the relationship between matrix porosity and permeability. One such possibility is the Carman-Kozeny equation [73],

$$k = k_i \frac{(1-\phi_i)^2}{(1-\phi)^2} \left(\frac{\phi}{\phi_i} \right)^3, \quad (44)$$

where all parameters are as previously defined, although matrix permeability is likely an insignificant contributor (in many cases) to overall system behavior.

3.9 Chemical strain and stress

Modifications in fracture aperture necessarily lead to changes in the local stress field. However, because FLAC^{3D} uses grid point displacements to calculate strains, see Eq.(4), and does not store values of strain, no provision is available to input strains due to aperture change and subsequently convert them into gridpoint displacements. An alternative method is needed.

For equally spaced orthogonal fractures, the impact of a change in aperture on local linear strain (unidirectional from a single fracture) is represented by,

$$\varepsilon_{CH} = \frac{\Delta b}{s}, \quad (45)$$

where s is fracture spacing and the subscript CH refers to the “chemical strain” component of total strain owing to aperture change. In the usual manner, total strain, ε , can be spectrally decomposed into components due to mechanical, M , chemical, CH , and thermal, T , behaviors as, $\varepsilon = \varepsilon_M + \varepsilon_T + \varepsilon_{CH}$.

Considering only thermal and chemical effects, the thermal/chemical

Fig. 7. Thermal loading/unloading cycle examining the effects of chemical strain. Parameters: $E = 13 \text{ GPa}$, $\nu = 0.22$, $\alpha_T = 12 \times 10^{-6}$.

strain is $\varepsilon_{TC} = \varepsilon_T + A$, where A is some constant representing the chemical portion. At incremental equilibrium we have $\varepsilon_{TC} = \alpha_T \Delta T + A$ which, upon rearranging, becomes,

$$\varepsilon_{TC} = \Delta T \left(\alpha_T + \frac{A}{\Delta T} \right), \quad (46)$$

Where $A = \Delta b/s$. This relationship provides a method to accommodate chemical strain by altering the coefficient of thermal expansion, α_T , in FLAC^{3D} at all nominal element volumes for respective aperture changes, and, as desired, maintains a non-linear dependence on temperature. However, because the function is undefined for temperature changes approaching zero, care should be taken in its application. In physical systems where aperture change, a strong function of the effective stress field, is dominated by thermal stress, such as geothermal systems, such strains will be tracked appropriately, but in systems that are nearly isothermal this method will be ineffective in transferring information to the mechanical system

(which may or may not be necessary, as isothermal systems are unlikely to experience chemical strain to the same degree).

3.9.1 Chemical strain in cyclic loading

Chemical strain is defined here as thermo-chemo-mechanically irreversible reduction in fracture aperture that results in a relaxation of stress in the surrounding rock. As illustrated in Fig. 1, this process is proposed to be of significant importance in fractured reservoirs and replicating it one of the primary goals of THMC modeling. To examine this process, we consider the case of a liquid saturated, high temperature and pressure fractured mass subjected to a complete cycle of thermal loading and unloading (Fig. 7). The model is a pseudo three-dimensional mass (unit width in z -direction, discretized in x and y) with zero-displacement boundaries and initially at a uniform 80°C , $\sigma' \approx 20.8\text{MPa}$. A high temperature (120°C) and pressure (2MPa above *in-situ*) source is placed at one end of the geometry ($x = 0$, $y = L/2$) with a low pressure source (2MPa below *in-situ*) at the opposing end ($x = L$, $y = L/2$), allowing the thermal source to translate across the geometry with the fluid pressure gradient. After thermal breakthrough to the injection temperature, the temperature source is reversed to 80°C , so that the mass then gradually declines to its initial temperature state. Progress is monitored at the central coordinate ($x = L/2$, $y = L/2$), and the results of temperature and aperture change versus stress at this location are displayed.

In the figure we present four cases incorporating different assumptions of response, which may be compared to the conceptual representation of Fig. 1. Fig. 7A is the baseline case, with completely reversible permeability change (Eq. (34) only), and no feedback of this chemical strain on the stress field (Eq. (46) not used). Fig. 7B represents the case of complete permeability constitutive treatment (Eqs. (34) and (41)) and includes feedback on stress field (Eq. (46)). Fig. 7C maintains full permeability constitutive treatment (as in 7B), but this time does not include feedback on stress (Eq. (47) not used). Finally, Fig. 7D considers complete reversibility (as in 8A), but this time includes feedback on the stress field (Eq. (47)).

The non-linear dependence of aperture on the temperature/stress field is evident, as is the non-linear dependence of stress on temperature that results from the feedback of chemical strain on the stress field. Two-dominant impacts on the system, hysteretic in nature, are visible by comparing the initial, ambient system with the final, ambient system. Importantly, when the system returns to its initial state, there has been an irreversible reduction in the stress field as well as an irreversible decrease in permeability. Neither of these occurrences, intuitively operative and significant in natural systems, may be represented without the inclusion of thermal, hydrologic, mechanical, and chemical processes.

3.10 Conclusions

A coupled THMC simulator has been developed with the capability to reproduce the undrained loading behavior of a fractured rock mass. Reactive transport has been included in the model via the equilibrium behavior of aqueous species (homogeneous reactions) and through kinetic considerations of mineral precipitation and dissolution. From multi-continuum hydrogeologic analysis, multi-phase fluid behavior is coupled to the mechanical response in one continuum via dual-porosity poroelasticity and thermodynamically controlled fluid compressibility. Permeability of the mass is followed with a new constitutive relationship representing thermal loading and unloading behavior: Closure of the fracture is controlled by thermal-elastic compaction and the dissolution of stress-concentrated asperities, while dilation occurs via thermal-hydraulic stress relaxation. Bulk permeability is also modified by the precipitation/dissolution kinetics of mineral species. The explicit coupling between THC and M behaviors is shown to reproduce the rapid response of a loaded mass.

Chemical strain is accommodated by the permeability constitutive relationship, and its impact on the stress field of a geologic environment is illustrated. For the first time, we present geologic scale numerical results illustrating the conceptual model that thermal loading may lead to an irreversible reduction in aperture and stress, so that the *in-situ* system may be completely altered by a cycle of loading.

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3.11 References

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4 CHAPTER 4: THERMAL-HYDROLOGIC-MECHANICAL-CHEMICAL PROCESSES IN THE EVOLUTION OF ENGINEERED GEOTHERMAL RESERVOIRS

Abstract

In a companion paper [1] we have introduced a new methodology and numerical simulator for the modeling of thermal-hydrologic-mechanical-chemical processes in dual-porosity media. In this paper we utilize the model to examine some of the dominant behaviors and permeability-altering mechanisms that may operate in naturally fractured media. Permeability and porosity are modified as fracture apertures dilate or contract under the influence of pressure solution, thermo-hydro-mechanical compaction/dilation, and mineral precipitation/dissolution. We examine a prototypical enhanced geothermal system (EGS) for the relative, temporal arrival of hydro-mechanical vs. thermo-mechanical vs. chemical changes in fluid transmission as cold (70°C) water is injected at geochemical disequilibrium within a heated reservoir (275°C). For an injection-withdrawal doublet separated by ~670m, the results demonstrate the strong influence of mechanical effects in the short term (several days), the influence of thermal effects in the intermediate term (<1 month at injection), and the prolonged and long-term (>1 year) influence of chemical effects, especially close to injection. In most of the reservoir, cooling enhances permeability and increases fluid circulation under pressure-drive. We observe thermo-mechanical driven permeability enhancement in front of the advancing thermal sweep, counteracted by the re-precipitation of minerals previously dissolved into the cool injection water. Near injection, calcite dissolution is capable of increasing permeability by nearly an order of magnitude, while precipitation of amorphous silica onsets more slowly and can completely counteract this increase over the very long term (>10 years). For the reinjection of highly-silica-saturated water, amorphous silica is capable of drastic reduction in permeability close to the injection well. With combined action from all mechanisms, permeability change varies by two orders of magnitude between injection and withdrawal. We illustrate the importance of the coupling between reactive transport and geomechanics. Mineral behaviors alter fluid flow paths and, in so doing, change the characteristics of thermo-hydro-mechanical aperture changes, and vice versa. We show how each incurs changes in the system that fundamentally alter the evolutionary paths of reaction and chemical/mechanical deformation in a manner that mandates the accommodation of process couplings for the full THMC suite of interactions.

4.1 Introduction

In enhanced geothermal systems (EGS), as in reservoirs for the sequestration of CO₂, radioactive waste repositories, petroleum reservoirs, and other subsurface engineered facilities, fluid circulation is influenced in both the short- and long-term by chemical reaction and thermal-hydro-mechanical deformation. These forces operate upon temporally dynamic and spatially variable fluid transport properties, such as permeability, porosity, and fracture interconnectivity.

There are many considerations in the design of EGS, and most relate to the behavior of fractures. These include the potential for short-circuiting, the evolution of heat transfer surface area and of fluid residence time, working-fluid losses, and larger environmental concerns such as induced seismicity. Many processes are active in this regard. Some *inhibit* fluid transmission in dominant fractures, such as thin-film pressure solution [2-6], mineral precipitation [7-9], and thermo-mechanical aperture closure or creep. Others *enhance* transmission, such as shear dilation [10,11], mineral dissolution, force of crystallization [12-14], and strain energy driven free-face dissolution [5-6], while shear and dilation on existing and growing fractures is considered the primary contributor to induced seismicity [15].

Simulating these behaviors currently requires a staged approach, with some of the behaviors encompassed in thermal-hydraulic (TH) or thermal-hydraulic-mechanical (THM) simulations, and others by thermal-hydraulic-chemical (THC) simulations. This may be adequate for many needs, but leaves out the rational and desirable linkage between chemical and mechanical behaviors. Pressure solution is by definition a chemical-mechanical process, as is free-face dissolution.

Other behaviors may, at first glance, seem adequately addressed through THM modeling, such as shear dilation and thermo-mechanical aperture closure. It is unclear, however, how such processes will be influenced by the action of chemical or chemo-mechanical mechanisms. For instance, aperture changes due to pressure solution result in the growth of contact area between fracture planes, and this in turn affects fracture shear strength and dilation angle. Alternatively, mineral precipitation/dissolution can alter the apertures of fractures, causing shifts in fluid and thermal flow paths that upset the stress condition and modify mechanical aperture. To examine these and other linkages, we introduce a modeling structure [1] that couples chemical and mechanical behaviors in a manner that reflects their interdependence on thermal and hydraulic effects (THMC). We apply this simulator to address some of the important questions in a prototypical EGS and, indeed, to examine the importance of these couplings and the strength of their interaction.

We first provide a brief overview of the approach and a description of the geological domain. A description of the chemical system and a simplified examination of injection water chemistry then follow

to set the stage for further analysis. This is followed by an assessment of the relative, temporal arrival of hydro-mechanical vs. thermo-mechanical vs. chemical changes in fluid transmission and a recast of these in terms of characteristic times. Next, and perhaps most importantly, we evaluate the necessity for the explicit coupling of reactive transport to geomechanical processes and quantify the strength of coupling between independent processes. Finally, we follow the evolution of deviatoric stress in the reservoir and indicate locations most likely to undergo shearing failure.

4.2 Simulation mechanism

The simulations presented in the following utilize a newly developed THMC simulator [16] that couples the multiphase, multi-component, non-isothermal thermodynamics, reactive transport, and chemical precipitation/dissolution capabilities of TOUGHREACT [7] with the stress/deformation analyses FLAC^{3D} [17]. The coupled model incorporates features unique to fractured reservoirs (particularly those under elevated temperature and chemical potential), involving the undrained pressure response in a dual-porosity medium and with chemo-mechanical effects on deformation and on transport.

This “modular” approach, first proposed by Settari [18] to couple geomechanics with reservoir flow simulation, has some advantages over the development of a single coupled program. Modular approaches take advantage of the high state of development, sophistication, and validation available in purpose-built codes. The appropriate linking of codes which represent different behaviors – in this case those of solid mechanics and fluid transport – enables complex coupled processes to be represented and their interaction explored. With the appropriate choice of linking parameters and with the use of flexibly defined mesh overlays, the interaction of complex coupled processes may be explored with reasonable confidence and with rapid development.

Additionally, the modular construction [18,19] allows for easier implementation of future advances in constitutive or modeling technology (rather than modifying an entire coding structure), although typically the codes are not optimized to perform interactively, and may execute slowly; in our experience lowering computational efficiency due to the time required for data transfer between modules. As suggested by Settari and Mourits [19] and Minkoff et al. [20], however, this may not always be the case, because in systems where geomechanics may be loosely coupled (not changing at a rapid pace) the geomechanics simulation may not need to be conducted very often, thus improving computational efficiency over fully coupled codes where mechanics are equilibrated at every fluid flow time step.

FLAC^{3D} is exercised purely in mechanical mode, where undrained fluid pressures may be evaluated (externally) from local total stresses. This undrained methodology allows calculation of the short-time build-up in fluid pressures that results from an instantaneous change in stress, provided we have

knowledge of the compressibility of the pore fluids and the solid matrix. In this way, the complex thermodynamics of phase equilibria of multiphase water mixtures, and even multi-component mixtures (such as CO₂ and water), can be tracked in the pre-existing framework of TOUGHREACT. For water mixtures, we utilize the 1997 International Association for the Properties of Water and Steam (IAPWS) steam table equations [21] to calculate fluid compressibility. If a system is unsaturated (such as in HDR) fluid compressibility is large, and the undrained poroelastic equations approach their drained counterparts. Therefore, while our construct is tailored to saturated systems, drained ones are automatically accommodated.

Sequential execution of the two programs is linked by a separate code, referred to as the “interpolation module”, capable of parsing data outputs from each primary simulator as input to the companion. This module is a Fortran 90 executable, and maintains access to data outputs from TOUGHREACT and FLAC^{3D}. In addition to data interpolation, the module executes constitutive relationships including permeability evolution, dual-porosity poroelastic response to stress, and thermodynamically controlled fluid compressibility.

4.3 THMC permeability changes

The modeling structure calculates permeability change from the combined action of pressure solution, thermo-mechanical dilation/contraction, hydro-mechanical dilation/compaction, and bulk volume precipitation/dissolution of mineral species, with each depending intrinsically on temperature, effective stress, and chemical potential. Several methodologies could be used to model these behaviors; in the following we utilize laboratory results of fracture behavior under hydrothermal conditions to constrain in a single constitutive relationship the first three mechanisms. Compaction of fracture asperities is governed by [20],

Table 1. Solid medium properties as used in simulations.

Parameter	Value	Parameter	Value
Bulk modulus of intact rock, $K^{(1)}$ (GPa)	17.0	Volume fraction of fractures (of total reservoir), θ	0.01
Composite bulk modulus, K (GPa)	8.00	Porosity within fractures, ϕ	0.3
Poisson's ratio, ν	0.22	Residual mechanical aperture, b_m^r (μm)	22.5
Bulk modulus of solid grains, $K_s^{(1)}$ (GPa)	54.5	Residual chemical aperture, b_c^r (μm)	20.0
Coefficient thermal expansion, α_T ($1/^\circ\text{C}$)	1.2×10^{-5}	Aperture change constant, β	1.11
Saturated thermal conductivity, λ (W/m·K)	2.9	Aperture change constant, χ	345
Heat capacity, C_p (J/kg·K)	918	Aperture stiffness constant, ω (1/MPa)	0.20
Porosity of porous media, ϕ	0.02	Mechanical recovery ratio, R_m	0.60

$$b_{mc} = b_m^r + \{b_m^r - b_c^r + b_m^{\max} \exp(-\omega\sigma')\} \cdot \exp(-\sigma'(\beta - \chi/T)) \quad (1)$$

where b_{mc} is the fracture aperture at a given temperature, T , and effective stress, σ' . The residual (minimum possible) aperture at extreme mechanical stress is given by b_m^r , and at extreme chemical stress by b_c^r . The maximum possible aperture change is $b_m^{\max}$ (or the difference between initial and residual aperture), and the empirical coefficients that must be fit to laboratory data are β , χ , and ω , and represent the chemical, thermal, and mechanical dependence of the aperture, respectively (with ω representing non-linear fracture stiffness). This relationship has been previously compared to laboratory data [16,22].

Unloading (gaping) of the fracture is controlled by [16, modified from 22],

$$b_{m(u)} = b_{mc}(\sigma'_{\max}) + R_m b_m^{\max} \{ \exp(-\omega\sigma') - \exp(-\omega\sigma'_{\max}) \} \quad (2)$$

where $b_{mc}(\sigma'_{\max})$ is the aperture at maximum loading (Eq. (1) evaluated at the maximum stress prior to unloading), and R_m is the recovery ratio (fraction of *mechanical* (not chemical) closure that is recoverable through mechanical-thermal unloading). This relationship implies that gaping of the fracture can only occur through mechanical-thermal elastic relaxation, and not through the chemical processes that influence closure in Eq. (1). The values of these parameters as utilized in our simulations appear in Table 1.

Chemical precipitation/dissolution is calculated within TOUGHREACT. The governing equations are described in Taron et al. [16], as presented in the works of Steefel and Lasaga [23] and Xu et al. [24]. Reactions between aqueous species (homogeneous reactions) are assumed to be at local equilibrium, and therefore governed by the relationship between the concentrations of basis (primary) species and their activities, partitioned by the stoichiometric coefficients. This relationship is termed the law of mass action [cf. 23]. The assumption of local equilibrium greatly reduces the number of chemical unknowns and ODE's (between primary and secondary species), and is accurate to the extent that the true reaction rates outpace the rate of fluid transport in a given system. This is a correct assumption for most aqueous species [23] (and flow systems), but less so for slower redox reactions [23,24]. In TOUGHREACT, species activities are obtained from an extended *Debye-Hückel* equation with parameters from Helgeson et al. [25].

4.4 Model results

In the engineered stimulation of geothermal reservoirs hydraulic, chemical [8,9,26,27], and thermal [28-31] means may be utilized to enhance permeability in a purposeful manner. These stimulations may be used to increase circulation in low permeability systems, and also to counteract future changes that occur as cold water is injected into the reservoir at geochemical disequilibrium. Ideally, injection and withdrawal wells will be connected by a fracture network that is sufficiently permeable to allow rapid fluid interchange, but impermeable enough to allow for sufficiently long thermal residence times in a medium with a large heat transfer area. In addition to achieving an appropriate balance between circulation and residence time, a natural concern arises as to whether unintended stimulations (resulting from critical thermo-hydro-chemical forces of injection) will generate short-circuiting paths between the injection and withdrawal wells via the modification of flow pathways through existing fractures.

Mineral scaling at the wellbore is a known problem, and recent work [e.g. 26,32] indicates that mineral precipitation may also play a large role in reservoir evolution. Moderate success (primarily for calcite) has been achieved in counteracting this through pH modification and the addition of chelatants [8,9]. Chemical changes and the effectiveness of chemical treatments, however, are coupled to hydro-mechanical fracture flow properties. At the Soultz-sous-Forêts geothermal site, for instance, productivity enhancement was observed from chemical treatment at two production wells, but had almost null impact at the injection well, presumably due to the presence of high conductivity fractures that transmitted the treatments quickly away from the problem area [9] and ameliorated their

Fig. 1. Initial conditions and geometric layout of EGS reservoir as used in simulations.

impact. The purpose of this work is to explore the chemical-mechanical couplings responsible for such behaviors and to quantify how strongly they are interlinked.

4.4.1 Characteristics of simulated EGS

We examine behavior in a prototypical EGS represented by a pseudo 3-D doublet geometry of $1500\text{m} \times 2900\text{m}$, with cold (70°C) fluid injected through a single well and extracted (670m away) through a single withdrawal well (Fig. 1). Initially, the reservoir is at 275°C . Horizontal stresses of 38.9MPa and a vertical stress of 61.7MPa are applied at time $t = 0^-$ and allowed to equilibrate with an initial pore pressure of 24MPa . These conditions are broadly representative of the east flank of Coso geothermal field [33,34]. The lateral boundary that crosses both the injection and withdrawal wells is a plane of symmetry, and as such is restricted to zero displacement in its orthogonal direction (roller boundary). Constant normal stress is held at all other boundaries, and every boundary is thermally insulated and impermeable. The fracture domain is given an initial (unstressed) permeability of $3.0 \times 10^{-11} \text{m}^2$, and the application of effective stress and temperature at $t = 0^-$ are allowed to decrease this permeability to an *in-situ*, equilibrium value via mechanical closure and pressure solution (assumed to have occurred slowly over geologic time prior to reservoir stimulation). This *in-situ* value is $6.8 \times 10^{-15} \text{m}^2$ at the given conditions. The granodiorite matrix is given a permeability of $2.0 \times 10^{-18} \text{m}^2$. Additional properties of the solid medium are shown in Table 1. The injection well operates as a constant source of pressure and temperature equivalent to a well diameter

Table 2. Initial volume fraction of reactive minerals in host reservoir. Remaining volume fraction (up to 1) is non-reactive.

Mineral	Volume fraction of solid rock ¹	
	Granodiorite	Fractured vein
Anhydrite	--	--
Anorthite	0.33	--
Calcite	0.02	0.31
Chlorite	--	0.23
K-Feldspar	0.17	--
Quartz	0.34	0.17
Amorphous Silica	--	--

¹From Kovac et al. [34]

of approximately 12 inches, while the withdrawal source serves as a single withdrawal well maintaining a constant pressure at the same diameter. The pressure differential is 3MPa above and below the *in-situ* value, respectively, and both enter the geometry at the boundary of symmetry.

Reactive composition of the host reservoir rock is presented in Table 2. Calcite and amorphous silica are expected to be the minerals primarily responsible for permeability change due to precipitation and dissolution [cf. 26,34]. Other likely minerals, such as potassium feldspar and quartz, are also followed, as listed in Table 2. Rate constants for precipitation/dissolution and mineral reactive surface areas of these common minerals are available in the literature, and were utilized as in Xu and Pruess [26]. Calcite and anhydrite are assumed to react at equilibrium (benefiting simulation time by lowering the *Damköhler* number). This assumption is warranted by their very fast relative rate of reaction.

4.4.2 Mineral precipitation/dissolution

Fluids that are injected into a geothermal reservoir are typically far from geochemical and thermal equilibrium with minerals in the host rock. As minerals precipitate from the injected fluid and dissolve from the rock, changes are incurred in the porosity and permeability of the fracture system. In currently operating geothermal systems, calcite and amorphous silica precipitation have posed problems at recovery and injection wells, respectively. Acidic injection has been shown to successfully inhibit calcite precipitation [8,15]. Aggressive acid-base reactions, however, tend to rapidly dissolve first-contacted minerals and lose effectiveness in the remainder of the wellbore [8]. Other problems with acidification include the potential for corrosion of steel casings, although corrosion inhibitors can often be used. Chelating agents, which reduce the activity of metal ions (through binding), are another alternative for calcite dissolution [9,35] that are suggested to have a less aggressive, more uniform effect [8,35].

Table 3. Fluid chemical compositions (*mol/l*) used in simulations. Reservoir composition is at time, $t = 0$. Injection fluid composition remains constant throughout simulation.

Chemical component	Reservoir fluid	Injection fluid		
		Water #1: Initial fracture vein water cooled and equilibrated at 70 °C	Water #2: Allowing only 80% completion of SiO ₂ precipitation during equilibration to 70 °C	Water #3: Restricting all mineral precipitation during equilibration to 70 °C
Al	8.520×10^{-3}	1.894×10^{-8}	1.894×10^{-8}	3.866×10^{-3}
Ca	1.020×10^0	1.976×10^0	1.976×10^0	1.976×10^0
Cl	7.420×10^1	1.074×10^2	1.074×10^2	1.074×10^2
Fe	4.531×10^{-9}	8.167×10^{-8}	8.167×10^{-8}	8.167×10^{-8}
HCO ₃	2.972×10^{-2}	2.010×10^{-1}	2.009×10^{-1}	2.010×10^{-1}
K	6.136×10^0	8.413×10^0	8.413×10^0	8.435×10^0
Mg	1.213×10^{-3}	3.938×10^{-3}	3.938×10^{-3}	3.938×10^{-3}
Na	6.359×10^1	9.255×10^1	9.255×10^1	9.255×10^1
SiO _{2(aq)}	6.210×10^0	4.549×10^0	4.881×10^0	7.856×10^0
SO ₄	2.766×10^{-2}	7.193×10^{-2}	7.193×10^{-2}	7.193×10^{-2}
pH	6.71	5.82	5.82	5.82

Inhibiting the precipitation of amorphous silica has proven more difficult [15]. HF treatment is currently the preferred method, but some have suggested that amorphous silica can be dissolved at high pH with the use of chelating agents to prevent calcite deposition (which would be favored at high pH) [8,35]. This research is, however, relatively recent, and uncertainty remains as to the effects of these treatments on the host rock. Geothermal environments are chemically complex, and field scale results are limited and mixed [9].

In the simulations that follow we present three scenarios for injection fluid composition. Injection water #1 is obtained by extracting the equilibrium, *in-situ* reservoir fluid at 275°C and allowing it to cool (not in the presence of reactive minerals, as if utilized at the surface with no treatment other than settling) to 70°C while the aqueous components equilibrate and minerals precipitate. For this injection water, our results show that the injection fluid is not sufficiently saturated with aqueous silica to incur significant reservoir precipitation of amorphous silica, although other minerals are very active. This is a result of the chosen chemistry. As a comparison, field measurements have shown that the precipitation of amorphous silica occurs in fractures at some injection locations in the Coso geothermal field (well 68-20RD), but not

at others (wells 68-20, 68A-20, 68A-20RD) [36], depending on the precise injection and *in-situ* chemistry at each well. Two alternative compositions are introduced to examine the behavior of amorphous silica precipitation. Injection water #2 assumes some inefficiency in the surface equilibration process (such as insufficient equilibration time or enhanced dissolution from turbulence) such that only 80% of potential silica precipitation occurs. Simulation #3 is further oversaturated in silica; it represents the potential for rapid chemical change in the reservoir and so assumes that mineral precipitation has been completely restricted during the cool down from 275°C to 70°C (only precipitation is restricted, as primary species are allowed to form secondary species in solution). Injection compositions for each of these cases and for the *in-situ* reservoir are shown in Table 3.

The mineral precipitation/dissolution results of our simulations utilizing these three injection waters are shown in Fig. 2. Fig. 2A compares each injection water for a simulation time of 5 and 20 years for the combined action of all minerals, while Fig. 2B illustrates results for injection water #2 and for each mineral individually. Units are cumulative change in mineral abundance (volume fraction) from time, $t = 0$, such that negative values represent dissolution. Values in Fig. 2B are normalized, such that multiplication of each curve by its normalization magnitude returns the units to cumulative change in mineral abundance. Importantly, water #1 exhibits net mineral dissolution near the injection well (where the cold injection water makes calcite dissolution highly favorable), and net precipitation outside of the thermal reach. This is desirable in the sense that the immediate injection area experiences an increase in permeability, but undesirable in that these dissolved minerals are then re-precipitated as they are heated again between the injection and withdrawal wells. Water #2 changes this behavior in a crucial manner; at five years the injection area still experiences net dissolution, but this magnitude is decreased by the precipitation of amorphous silica, and at 20 years the action of amorphous silica has completely erased the positive influence of calcite dissolution. Water #3 shows a more dramatic result, where silica precipitation completely dominates the injection area. This behavior is so pronounced that the simulation was ceased after 7 years due to a complete shutdown of injection permeability ($<10^{-18} \text{ m}^2$), and so only the five year value is plotted in the figure. One final point regards the magnitude of mineral precipitation outside of the injection area. The higher hydraulic gradient between injection and withdrawal partially outpaces mineral precipitation, such that there is a higher buildup of deposited minerals on the opposite side of injection due to a lower fluid velocity (higher *Damköhler* number).

Fig. 2. A.) Change in mineral abundance (all minerals combined) at 5 and 20 years for each of the three injection compositions. Negative values indicate dissolution (decrease in the solid volume fraction). B.) Behavior of each mineral utilizing water #2. Each curve normalized to its own maximum value: Number beneath each mineral indicates the normalizing value (multiply by this number to obtain the true value of each curve).

Further parametric analyses of injection chemistry are not addressed here [cf. 7, 8, 34, 36]. The primary interest in what follows is to present an analysis *not* of specific chemical changes, but of how these changes impact the mechanical system, and how feedback from other permeability altering mechanisms may shift chemical behaviors. We begin by examining the competing magnitudes of chemical vs. hydraulic vs. thermal effects.

4.4.3 Temporal permeability change

Our model so far attempts to interlink the most important mechanisms in the alteration of reservoir fluid transport properties. This section reverses direction and attempts to extract from the coupled analysis the magnitude of influence for each process. It is of interest, both for overall reservoir evolution and for

evaluation of potential hydraulic/chemical stimulations, to observe the temporal onset of the various mechanistic causes: In what stages of the lifespan of a geothermal project is thermal (or chemical or hydraulic) forcing the dominant mechanism for change? What measures could then be taken to counteract this, and when should they be applied?

A conceptual model for the possible temporal relationships between THMC processes is shown in Fig. 3A. In a geothermal reservoir subject to cold water injection, hydraulic stimulation should have an immediate effect, tapering off with time to a steady long-term influence. Thermal effects would exhibit a similar trend, but the thermal transfer rate would greatly slow the onset of changes, and there would perhaps be slight reversibility following passage of the thermal front (as adjacent grid blocks contract). Chemical effects should act even more slowly, and perhaps have a dominant influence in the extreme long-term of reservoir life. Mechanical effects are directly active in the first two of these processes – through effective stress and thermal stress.

Simulation results are presented in Fig. 3B in a manner analogous to the conceptual model of Fig. 3A. Aperture change is monitored at three locations in the reservoir (2m, 9m, and 49m outward from injection), and each curve at each location represents the contribution of a different process. Total aperture change refers to the contribution from all mechanisms and so reflects the observable change in permeability. Also shown is the contribution to total permeability change due to mineral precipitation/dissolution and thermal-hydraulic processes (asperity dissolution via pressure solution and thermal gapping due to cooling). For asperity dissolution/thermal gapping, behavior is conditioned by the combined influence of effective (not total) and thermal stress, and so in this analysis hydraulic and thermal effects cannot be separated (although we present some separation in terms of characteristic times in the following section).

Some clarification is helpful in regard to the two processes implied by thermal-hydraulic. In our pressure solution model (see Section 3 and Taron et al. [16]), fracture gapping is not allowed via chemical means (“force of crystallization” is not considered), but only occurs through thermo-mechanical-hydraulic unloading. This behavior, however, is not simply calculated via thermal shrinkage of the matrix blocks, but is handled constitutively as a function of stress reduction and temperature change at the fracture face, and is therefore calculated from the empirical closure relationship (Eqs. 1 and 2). When the reservoir is loaded, pressure solution is active and instantly (numerically) reduces the reservoir permeability to its “initial” state at loaded conditions (assumed to have occurred

Fig. 4. Plan-view distribution of logarithm of permeability (filled contours) and isotherms (empty dashed contours) at 20 years using water #2. Isotherms increment by 30°C from 70°C to 250°C.

slowly over geologic time before stimulation of the reservoir). As the reservoir cools, the matrix contracts and most areas of the reservoir experience thermo-mechanical gapping, while some areas experience an increase in stress and a continuation of pressure solution creep. Both of these actions are controlled by the constitutive relationship, and because thermal gapping is the dominant mechanism during cooling, we refer to both with the thermal-hydraulic curves in Fig. 3B.

Mineral precipitation/dissolution is represented by the dashed lines in Fig. 3B. At points near injection, permeability is increased significantly in early times as calcite dissolves into the cool injection water; this behavior is not visible at 49m from injection. During this time, amorphous silica precipitation counters the dissolution of calcite and decreases permeability, but this behavior is not visible in the plot due to strong dominance from calcite dissolution. As time proceeds, silica is more successful at decreasing permeability and after 5.2 years (2m from injection) and 17.5 years (9m from injection) nearly all of the existing calcite within fractures has been dissolved and amorphous silica overrides as a net decreasing trend in permeability. Note that in this simulation calcite dissolves at equilibrium, and that the introduction of kinetic constraints could partially shift the behavior of calcite. At 49m from injection, only precipitation is significant during the first 20 years of simulation. Note also that neither anhydrite or anorthite is shown in the figure; their contribution is smaller by several orders of magnitude and is focused on the edge of the thermal front $\geq 100m$ from injection.

Fig. 5. Permeability changes using water #2. A.) Total permeability change with distance from injection. B.) Mineral precipitation/dissolution portion and thermal-hydraulic portion of total permeability change in (A). Note the change of scale on the x-axis of (B).

Fig. 4 shows contours of permeability and temperature for a reservoir plan-view after 20 years of simulation. Note that the highest permeability is at the injection well, and this tapers off to either side and is surrounded radially by a pocket of lower permeability, particularly to the opposite side of withdrawal. Fig. 5 shows permeability change at a cross section between wells. Note the nearly two order of magnitude variability, and the development of a radial barrier of lower permeability approximately 50m outward from injection. Fig. 5B illustrates more clearly how this barrier corresponds to the re-precipitation of minerals that are dissolved at injection.

4.4.4 Characteristic times

We can further elucidate the time dependency of competing mechanisms by plotting them versus their respective characteristic times. We thus introduce the characteristic time, $t_D = ct/l^2$, at a time, t , over the characteristic length scale, l . The diffusivity, c , refers to the ratio of conductivity to capacity/storage, and for thermal conductance is represented by thermal conductivity of saturated rock, λ , density, ρ , and heat capacity, C_p , as $c_T = \lambda/\rho C_p$. When examining the characteristic thermo-elastic response of the reservoir, we note that the timescale of thermal expansion due to a change in temperature will be nearly instantaneous in comparison to the rate of thermal/hydraulic transfer that allows such a temperature change. Hydraulic transport will also influence the thermal characteristic time, such that cooler fluid will be transported via the fracture network to the characteristic location before being thermally conducted into the rock matrix. We conceptualize this process as two conductors in series; thermal characteristic time is recast as $t_D = t \cdot c_{TH}$, where c_{TH} is thermo-hydraulic diffusivity and includes hydraulic and thermal effects as, $1/c_{TH} = l_T^2/c_T + l_H^2/c_H$, where the thermal characteristic length scale, l_T , is fracture spacing and the hydraulic length scale, l_H , is the distance of the characteristic location from the injection well. Hydraulic diffusivity, c_H , is discussed below.

Hydraulic effects are characterized by the poroelastic fluid diffusivity, $c_H = k/\mu S$, for permeability, k , dynamic viscosity, μ , and 3-dimensional storage coefficient, S (see Wang [37] page 55 for a discussion of storage coefficients), defined as,

$$S = \frac{1}{K_v} + \frac{\phi}{K_f}, \quad (3)$$

for the effective porosity of the fractured medium, ϕ , fluid bulk modulus, K_f , and for the solid modulus, $K_v = K + 4/3G$, where K and G refer to the bulk and shear modulus, respectively. Again, the solid response to pressure change is much faster than the rate of fluid conductance, and so the hydraulic poroelastic response is characterized by this hydraulic diffusivity.

For chemical effects, we introduce an analogous relationship. Whereas before we were interested in the ratio of transport to storage, chemical effects depend on the relationship between the rate of chemical reaction and the storage capacity of chemical species in the fracture system. This gives the chemical characteristic time as the ratio of chemical reaction rate to volume capacity of the fractures,

$$t_D = \frac{k_R S_A}{(\theta \phi V/V_M)} \cdot t, \quad (4)$$

for the reaction rate, k_R (in $mol/m/s$), total area of precipitation/dissolution (fracture surface area), S_A , volume fraction of fractures in the reservoir, θ , porosity of these fractures, ϕ , characteristic volume scale, V , and molar volume of the mineral species, V_M . We can also rearrange this relationship to produce a “chemical diffusivity” analogous to the above relationships, $c_C = k_R S_A / (\theta \phi h / V_M)$, for reservoir width in the z-direction, h , so that the characteristic time retains its form as $t_D = c_C t / A$, for the characteristic reservoir area, $A = \pi l_c^2$, for the characteristic length, l_c , which is the distance of the characteristic location from the injection well. We thus obtain three characteristic times (and diffusivities) to represent the thermal, hydraulic, and chemical aperture response.

In Fig. 6, four characteristic areas are examined within the influence field of injection; one of 9m characteristic length (encompassing the area closer than 9m from injection), one of 24m, one of 49m, and one of 129m, and we take 70°C (corresponding to the water injection temperature) to be the dominant temperature condition for the life of the project (within these characteristic areas). Water properties correspond to this temperature, and reaction rate is adjusted to this temperature via the Arrhenius expression,

$$k_R = k_{25} \exp \left(-\frac{E_a}{R_u} \left(\frac{1}{T} - \frac{1}{298.15} \right) \right), \quad (5)$$

for the gas constant, R_u , activation energy, E_a , and the rate constant at 25°C, k_{25} .

As mentioned above, asperity dissolution/thermal gapping behavior is conditioned by effective (not total) and thermal stress and so hydraulic and thermal effects are not directly separable. However, we can focus on hydraulic effects by extracting from the simulation data any changes that occur prior to any noticeable change in temperature; because hydraulic effects are deduced to occur well in advance of thermal arrival. This pre-thermal onset time varies from approximately 10 minutes at 9m from injection to 4 days at 129m from injection. Closer than 9m from injection we are unable to distinguish between mechanisms. Fig. 6 separates hydraulic and thermal effects (both contributing to the empirical aperture change relationship) via this observation, so that data points prior to this shift in behavior are

Fig. 6. Characteristic times of permeability change due to hydraulic, thermal-hydraulic, and chemical mechanisms. Changes monitored at 9 m, 24 m, 49 m, and 129 m from injection. Uses water #2.

assumed to relate to hydraulic influence (and become the hydraulic curve in Fig. 6). Because the thermal-mechanical relationship includes the effect of hydraulic diffusivity (see above), no separation is required here and the curve is plotted from time, $t = 0$ (this is the true thermal-hydraulic curve). To examine characteristic chemical behavior, we adopt for simplicity the rate constant and activation energy of amorphous silica precipitation.

From Fig. 6, we note that for the three plots (hydraulic, thermal-hydraulic, and chemical), most of the changes fall characteristically within a timescale of $t_D \approx 1.2$. Ideally, a curve at any location would overlay

perfectly with any other location by characteristic scaling. Given the strong couplings expected between each of the three mechanisms, however, it is perhaps surprising to observe any tendency to follow this ideal, particularly for the thermal-hydraulic curves.

In addition to providing a general picture of characteristic reservoir changes, this analysis would seem to have implications for the strength of coupling between each mechanism: a perfect overlay of all curves could indicate a weak coupling. For instance, that thermal-hydraulic effects do not significantly influence chemical trends, such that reactive transport simulations at invariant stress would not suffer a penalty in accuracy for this assumption. The following section presents a more direct analysis of this coupling strength.

4.4.5 *Strength of coupling*

The primary justification for a THMC modeling strategy is that there exists a strong coupling between chemical and mechanical effects that cannot be represented by parallel reactive transport and geomechanics simulations. In this section we examine the truth of this assertion. We first note that pressure solution can only be simulated with chemo-mechanical coupling, and this alone provides partial justification. However, in the current equilibrium based pressure solution model, coupling to a reactive transport framework is not required (such a linkage may be desirable, but its necessity is currently unclear). Further justification of coupling strength is desirable.

By examination of Figs. 3-5 it is clear that both reactive transport and geomechanical (THMC asperity dissolution/dilation) analysis are required to reproduce the observed order of magnitude changes in permeability; with each causing changes at least as large as one order of magnitude. Furthermore, our pressure solution relationship reduces initial permeability from $3 \times 10^{-11} \text{ m}^2$ to $6.8 \times 10^{-15} \text{ m}^2$ at *in-situ* reservoir conditions (this initial drop is not shown in the figures). Therefore, both of these methodologies are important, and both are required to follow reservoir behavior under these prototypical EGS conditions; but this conclusion does not necessarily imply that they must be interlinked.

Fig. 7 examines this necessity. Fig 6A and 6B show permeability changes *due only to mineral precipitation/dissolution* (from an initial value of $6.8 \times 10^{-15} \text{ m}^2$). Two different line styles represent two different simulations; the first utilizes our coupled THMC scheme, and the second operates under invariant stress (no mechanical equilibration and thus no pressure solution or thermal-mechanical dilation). Therefore, differences between the two simulations indicate shifts in mineral precipitation/dissolution behavior that are *caused by changes in the mechanical system*. In Fig. 7A, at 50m to the left of injection, a reactive transport simulation shows that

Fig. 7. Permeability comparisons for degrees of coupling. A.) Permeability changing due to mineral precipitation/dissolution only: Compares full coupling vs. reactive transport alone (invariant stress, no stress dependent aperture change). B.) Same as (A), versus time. C.) Permeability changing due to pressure solution/thermal dilation only: Compares full coupling vs. exclusion of reactive transport. D.) Same as (C), using water #3 (all others use water #2).

mineral behaviors cause a reduction in permeability from $6.8 \times 10^{-15} \text{ m}^2$ to $5.4 \times 10^{-15} \text{ m}^2$, while the coupled THMC simulation shows a drop to $2.3 \times 10^{-15} \text{ m}^2$, or a 3-fold increase in the amount of permeability occlusion, while 10m to the left of injection shows a 3-fold increase in permeability enhancement. At injection, there is further evidence of this, where amorphous silica precipitates more rapidly in the THMC coupling, resulting in a lower final permeability. Fig. 7B plots these same simulations versus time, and again illustrates the strong dependence of mineral reactions on mechanical changes.

Fig. 7C and 7D invert the comparison to examine how changes in the chemical system may alter the evolution of mechanics. Here we plot permeability change *resulting only from* pressure solution/thermo-mechanical gapping, with the same initial value as before. The lines again represent two simulations; one

THMC coupled, and a second that does not allow chemical reaction. Therefore, differences between the two simulations indicate shifts in the thermal-

Fig. 8. Plan-view of reservoir with deviatoric stress contours (in MPa) at 5 and 20 years of simulation. White lines are oriented as orthogonal to minimum principal stress direction, and are scaled to the magnitude that shear stress exceeds shear strength.

mechanical system *caused by changes in the chemical system*. In Fig. 7C we again see shifts in pressure solution/thermal dilation that are caused by precipitation/dissolution, but the coupling is not as strong as for the inverse condition in Fig. 7A. To examine the potential for greater coupling, Fig. 7D conducts the same simulation but utilizes water #3 (more chemically rich). In this case, very large, order of magnitude differences in thermal-mechanical dilation occur when chemical reaction is included.

4.4.6 Evolution of stress

Deviatoric stress that arises around thermal input can alter fluid circulation and generate a microseismic response. When the deviatoric stress exceeds the bulk strength of reservoir rock or existing fracture planes, permeability may be increased through the dilation and/or extension of existing fractures. This

will alter fluid flow paths, and introduce the potential for microseismicity. Fig. 8 follows the advance of deviatoric stress ($\frac{1}{2}(\sigma_1 - \sigma_3)$) with shaded contours. Included on the plot are white vectors to indicate locations where shear stress currently exceeds the reservoir shear strength at that location, and they scale with the excess stress to strength ratio. Their direction indicates the likely direction of failure were it to occur (orthogonal to minimum principal stress). Shear strength is calculated based upon an internal angle of friction of 25 degrees and zero cohesion.

4.5 Conclusions

A new simulator is utilized to examine dominant permeability altering mechanisms as they relate to critical thermal, hydraulic, mechanical, and chemical behaviors in a prototypical geothermal reservoir. Results demonstrate the strong influence of mechanical effects in the short term, the influence of thermal effects in the intermediate term, and the prolonged and long-term influence of chemical effects. THMC changes are recast in terms of respective characteristic times, where changes in fracture aperture are shown broadly represented by diffusive timescales representing the respective T, H, and C processes. The potential is evident for permeability alteration of several orders of magnitude due to thermo-hydro-mechanical dilation and chemical precipitation/dissolution. These two processes compete to dominate reservoir behavior; the former controlling the short-term response, and the long-term response characterized by the latter. For the injection of silica saturated water, amorphous silica is capable of drastically reducing permeability close to the injection well. This influence may be countered by the evolution of mechanical shearing in the near-well region, which may exert a strong influence on reservoir and characteristic behavior. Its inclusion into the modeling structure will be the focus of a future work. As an entry point to such an analysis, we have illustrated potential locations for reservoir shear failure by following the evolution of deviatoric stress and its relationship to thermally-derived shear stress.

We have also taken a first step towards the primary justification for a THMC modeling strategy; that there exists a strong coupling between chemical and mechanical effects that cannot be represented by parallel reactive transport and geomechanics simulations. We provide evidence in support of this assertion, illustrating how mineral behaviors alter fluid flow paths and, in so doing, change the characteristics of thermo-hydro-mechanical aperture changes, and vice versa. We show how each incurs changes in the system that fundamentally alter the evolutionary paths of reaction and chemical/mechanical deformation in a manner that decreases the accuracy of conducting the simulations separately.

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5 PUBLICATIONS AND PRESENTATIONS

5.1 Journal Articles

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6. Faoro, I., Elsworth, D., Marone, C.J., Niemeijer, A.R. (2006) Effect of Shear and Deviatoric Stress on Permeability Evolution in Fractured Diorite and Novaculite *Eos Trans. AGU, 87(52), Fall Meet. Suppl., Abstract S33A-0221*
7. Taron, J., Min, K.-B., and Elsworth, D. (2006) Simulating Thermal-Hydrologic-Mechanical-Chemical Evolution Surrounding Fluid Injection in a Fractured Porous Geothermal Reservoir. *Eos Trans. AGU, 87(52), Fall Meet. Suppl., Abstract NG54A-06*
8. Elsworth, D., Yasuhara, H., Liu, J., Polak, A., Grader, A., Halleck, P. 2005. Constrained observation of stress- and chemistry-mediated changes in the transport properties of fractured rock via physical and chemical signals supplemented by X-ray CT. Invited. *EOS AGU Trans. (Dec AGU Mtg).*
9. Yasuhara, H., Polak, A., Elsworth, D., Grader, A., Halleck, P. 2004. Enigmatic Permeability Switching in Fractures Under Net Dissolution. *EOS AGU Trans. (Dec AGU Mtg).*

5.4 Selected Invited Presentations

1. Elsworth, D. 2008. Stress- and chemistry-mediated changes in the transport properties of porous and fractured reservoir rocks. ExxonMobil Upstream Research Company. Houston, TX. August 20. [Invited]
2. Elsworth, D. 2008. Coupled physiochemical effects in the evolution of subsurface reservoirs – when they don't do what you want them to do! Department of Geosciences, University of Arkansas, Fayetteville, Arkansas, February 20. [Invited]

3. Elsworth, D. 2007. Coupled effects - THMC. International DUSEL Workshop. 11th Congress of Int. Soc. For Rock Mechanics. Lisbon, Portugal. July. [Invited]
4. Elsworth, D., Flemings, P.B., Marone, C.J., and Saffer, D.M. 2007. Activities in Rock and Fluid Physics at G³.
 - a. Shell Development Corp., Houston
 - b. Exxon Mobil, Houston.
 - c. BP Amoco, Houston.
 - d. Chevron Texaco, Houston.
5. Elsworth, D., and Fairhurst, C. 2007. Some opportunities for science and engineering at DUSEL. Proc. Can-US Symposium on Rock Mechanics. Vancouver, BC. May. [Invited]
6. Elsworth, D. 2007. Integrated active experimentation and modeling studies to probe the mechanical and transport properties of fractures. Workshop on Microbially Enhanced Oil Recovery, University of Western Australia, Perth, Australia. May 24. [Invited]
7. Elsworth, D. 2007. Evolution of the Mechanical and Transport Properties of Fractures: Interactive Feedbacks of Stress and Chemistry. SIAM Conf. on Mathematical and Computational Issues in the Geosciences. Santa Fe, MN, March. [Invited]
8. Elsworth, D. 2006. Stress- and chemistry-mediated permeability enhancement in critically-stressed fractures. DOE-EGS Program Review Meeting, Golden, Colorado, July.
9. Liu, J., Sheng, J.C., Zhu, W.C., Elsworth, D., Liu, J.X., Liao, Q.L., and Brady, B.H.G. 2006. Effects of heterogeneity on the multiphysics of fractured rocks. Proc. GeoProc 2006. [Keynote Lecture].
10. Elsworth, D., Yasuhara, H., Liu, J., Polak, A., Grader, A., Halleck, P. 2005. Constrained observation of stress- and chemistry-mediated changes in the transport properties of fractured rock via physical and chemical signals supplemented by X-ray CT. EOS AGU Trans. (Dec AGU Mtg).
11. Elsworth, D. (2005) Stress- and chemistry-mediated changes in the mechanical and transport properties of porous and fractured rocks: observations and some unanswered questions. Annual Meeting of the Geothermal Research Society of Japan, Obama, Nagasaki, Japan, November.
12. Elsworth, D. (2005) Stress- and chemistry-mediated changes in the mechanical and transport properties of porous and fractured rocks: observations and some unanswered questions. Third International Workshop on Water Dynamics, Sendai, Japan, November.
13. Elsworth, D. (2005) Stress- and chemistry-mediated changes in the mechanical and transport properties of porous and fractured rocks: observations and some unanswered questions. ExxonMobil Research and Engineering, Annandale, New Jersey, July 26th.
14. Elsworth, D., Yasuhara, H., Polak, A., and Liu, J. (2005) Short timescale chemo-mechanical effects and their influence on the transport properties of fractured rock. Keynote lecture. Proc. 11th International Conference on Computer Methods and Analysis in Geomechanics. Turin, June. Vol. 3 pp. 517-530.
15. Elsworth, D. and Yasuhara, H. (2005) Stress- and Chemistry-mediated Permeability Enhancement/Degradation in Stimulated Critically-stressed Fractures. Energy and Geoscience Institute, University of Utah, January 10, 2005.
16. Elsworth, D., Polak, A., Yasuhara, H., and Grader, A. (2004) Coupled chemical-mechanical effects and their influence on the transport properties of fractures in rock. Invited lecture. Symposium on

Flow and Transport: Characterization and Modeling from Pore to Reservoir Scales. DoE Office of Basic Energy Sciences. Gaithersburg, MD. September.

17. Elsworth, D. and Yasuhara, H. (2004) Short-timescale chemo-mechanical effects and their influence on the transport properties of fractured rocks. Keynote lecture. Euro-Conf on Rock Physics and Geomechanics. Potsdam. Germany. September.
18. Elsworth, D. (2004) Deep underground science and engineering program – planning and technical requirements: geo-engineering perspectives/needs. Plenary lecture. Workshop on Deep Underground Science and Engineering, Berkeley, CA. August.

5.5 Graduate Theses

1. Faoro, Igor. Evolution of Mechanical and Transport Characteristics of Fractures in Novaculite and Diorite. M.S. Thesis. 70 pp. Energy and Geo-Environmental Engineering, The Pennsylvania State University, University Park, Pennsylvania (2006).
2. Yasuhara, Hideaki. Thermo-Hydro-Mechano-Chemical Couplings that Define the Evolution of Permeability in Rock Fractures. Ph.D. Thesis. 259 pp. Energy and Geo-Environmental Engineering, The Pennsylvania State University, University Park, Pennsylvania (2005). [Hide Yasuhara received ARMA's 2006 N.G.W. Cook Ph.D. Thesis Award, and ISRM's 2007 Rocha Medal for this contribution.]