The Interplay between Geometry and THMC Processes

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ABSTRACT: Earth systems consist of materials with complex geometric features undergoing complex coupled thermal-hydro-mechanical-chemical (THMC) processes. These geometric features when combined with THMC processes govern the formation and transformation of rocks and thus understanding this coupling is essential for rock engineering activities. In this paper, we aim to address the following scientific questions by presenting a series of examples from numerical modeling and laboratory experiments: (1) How does fracture asperity geometry affect compaction and shearing that control single-fracture mechanical and flow properties? (2) How do intersections of fractures affect deformation, fluid flow and chemical reaction? (3) What controls key processes such as pressure solution during the formation of sedimentary rocks? Through these examples, we will show that it is important to properly address the complex geometry and coupled processes to understand evolving Earth systems to maximize their potential use for energy recovery and storage.

Keywords: Geometry, THMC, Fractures, Interfaces, Pressure Solution, Earth Systems.

1 INTRODUCTION: FRACTURE AND INTERFACES IN EARTH SYSTEMS

Earth systems are unique because they are stressed, fluid-filled, and heated. Materials within Earth systems consist of a variety of minerals and structures that respond differently to coupled processes, and these minerals form porous, fractured, granular systems at distinct scales. Understanding the role of coupled processes in the formation and evolution of these structures, from microscale structure to core-scale samples, is of critical importance for the prediction of the meso- to macro-scale multi-physical geosystem behavior, thus providing effective control of subsurface energy recovery and storage activities such as hydrocarbon recovery, geothermal energy, and nuclear waste disposal.

In Earth systems, three types of interfaces are ubiquitous: fluid-fluid, fluid-solid and solid-solid interfaces (Knight et al. 2007). At the pore scale, the fluid-fluid interfaces can often be described by curvature, and movement of fluid-fluid interfaces play a key role in the flow and displacement of CO2/H2/oil that affects the storage and recovery in the subsurface. Fluid-solid interfaces, affected by solid surface geometry (e.g. roughness), determines adsorption and reactive surfaces, however, these surfaces can be modified by chemical reaction via dissolution and precipitation (Steefel & Hu

2022). The most complicated interfaces are perhaps the solid-solid interfaces that can be arbitrarily shaped, distributed and modified because of THMC processes. The interaction of these solid-solid interfaces includes fracture/faults at the meter scale that determines the safety of gas storage and waste disposal and are the key component in reservoir recovery. At the tectonic scale, these solid-solid interfaces define the mechanical stability of tectonic plates driven by geothermic activities and further determine the availability of geothermal resources to human society on the Earth.

Fractures exhibit different geometrics features at different scales. At the reservoir and outcrop scales (m-km), fractures appear in networks, arbitrarily intersecting with each other. At the core scale (mm-cm), a dominant fracture may contain mineral fillings and may be connected to smaller fractures in the surrounding rock. On the microscale (1 mm-1 cm), a single fracture is basically the connected failure paths along, between or through individual mineral grains (Hu & Rutqvist 2022).

In this paper, we aim to address the following scientific questions by presenting a series of numerical modeling and laboratory experiments in the next sections. Those include examples to show (1) impacts of fracture asperities on deformation (Hu & Rutqvist 2020), (2) impacts of fracture intersections on deformation (Hu & Rutqvist 2022 and Santos et al. 2022), and (3) pressure solution occurred at different stages during the formation of sedimentary rocks (Hu et al. 2021 and Hu et al. 2022).

2 COUPLED GEOMETRY AND THMC PROCESSES IN EARTH SYSTEMS

2.1 Impacts of Fracture Asperities on Deformation

To understand the effect of asperities on deformation, we calculated mechanical deformation of rough fractures with explicit representation of the asperities with lateral confinement (Hu & Rutqvist 2020). Here we show three different profiles of asperity geometry and distribution: (1) evenly distributed smaller asperities, and (2) non-uniformly distributed asperities with two major asperities.

Figure 1 shows the results of vertical and shear stresses for each case. As can be seen, both the vertical stress and the shear stress are evenly concentrated at the contacting areas along the fracture for case (1), whereas for cases (2) and (3) the dominant contacting asperities govern the closure as well as stress concentrations. Such a high stress concentration for cases (2) and (3) could lead to a number of responses such as fracture initiation, plastic deformation, or pressure solution if the chemical-mechanical conditions are satisfied.

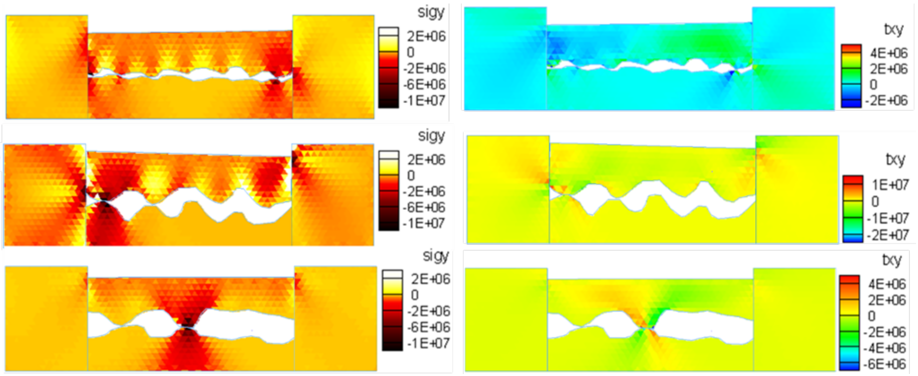

Figure 1. Calculated normal (left) and shear (right) stresses (Unit: Pa) of a compressed fracture when reaching equilibrium. From top to bottom: Cases (1), (2) and (3). (Hu & Rutqvist 2020).

From these examples, we demonstrate that the dominant asperities, which may not be captured by any statistical function, govern the closure and stress of a rough fracture. Thus, an empirical nonlinear function that describes normal stiffness of rough fractures should be used with caution because the details on how the contacting asperities are spatially distributed affect fracture stiffness (Kendall & Tabor 1971 and Hopkins 1991) and predictions of fluid flow (Pyrak-Nolte & Nolte 2016).

2.2 *Impacts of Fracture Intersections and Asperities on Deformation*

2.2.1 *Shearing of Two Intersecting Planar Fractures*

Here we examine three different scenarios of two intersecting fractures with orientations of 60° and −60°, and 45° and −60° (as shown in Figure 2, top row). The bottom of the domain is fixed, while a vertical loading of 10 MPa is applied on the top. On the left and right boundaries, horizontal loadings of 5 MPa are applied. We simulated the shear displacements of each fracture in each scenario and compared the results of the shear displacement to the analytical solution (Pollard & Segall 1987) where only the shearing of a single fracture is considered. The purpose of this comparison is to show the impact of the intersection on each single fracture by showing the deviation in shear displacements from the analytical solution from the single fracture case. The results are shown in Figure 2 (bottom row). Note that the sizes of these domains (i.e., the relative size of each domain to the length of the fractures) is carefully selected based on single-fracture modeling to eliminate boundary effects (Hu & Rutqvist 2022).

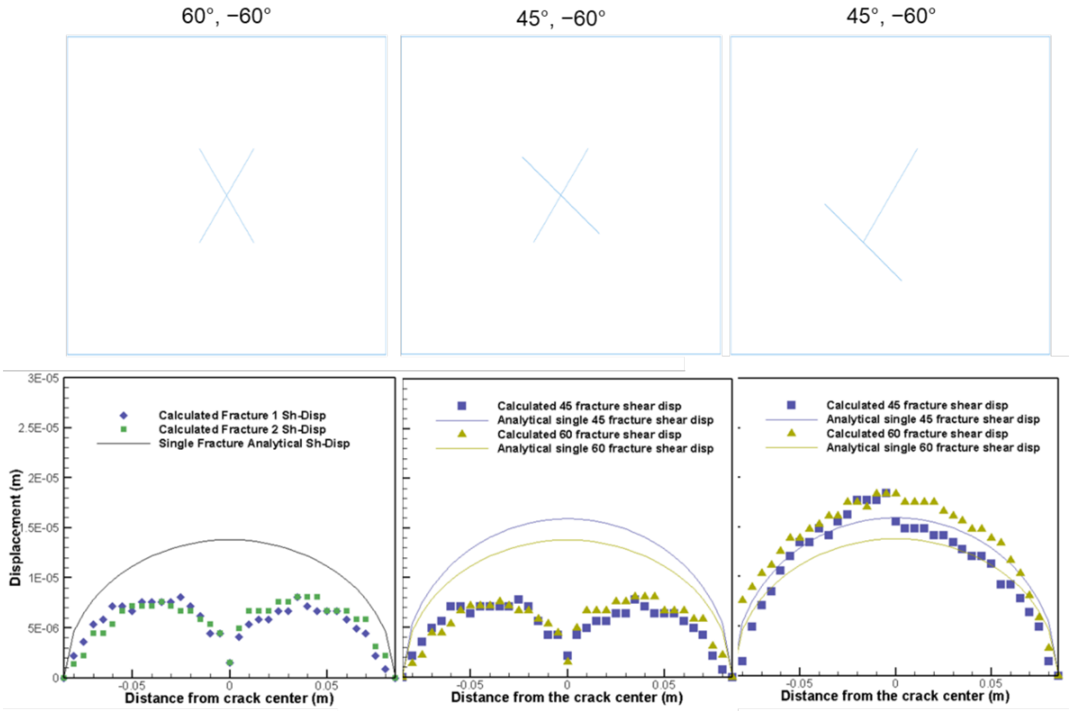

Figure 2. Three scenarios of geometry (top row) and NMM calculated shear displacements (bottom row) of two intersecting fractures with orientations of 60° and −60° (left), 45° and −60° (middle and right).

As shown in Figure 2 (bottom row: left and middle), when two intersecting fractures cut through each other (60° and −60° and 45° and −60°), each fracture is divided into two sub-fractures and shearing of either fracture is prohibited at the intersection. If the 45° fracture intersect with the −60° fracture only intersect at the tip of the −60° fracture (Figure 2, right), the distribution of the shear displacement of the −60° fracture exhibits similar results to that of a single −60° fracture with values larger than average. The 45° fracture shows a jump in the displacement adjacent to the intersection whereas the other part of the 45° fracture remains almost undisturbed by the intersection.

2.2.2 *Deformation of Two Intersecting Rough Fractures*

The impact of intersections on fracture deformation is further complicated when the fractures are rough, and the asperities are not negligible. The orientation relative to applied stress field affects the deformation, geometry, and connectivity of fracture networks. 3D X-ray microscopy was used to image the deformed geometry of two simple fracture networks (Figure 3). Connectivity was maintained in the "+" intersecting fractures by the vertical fracture that remained opened. The void volume of the horizontal fracture decreased significantly compared to the vertical fracture. For the "X" orientation, the shear displacement at the fracture intersection affected the connectivity of the network, with only a few tenuous connected flow paths across the intersections. Note how the topology varies from "X" to "V" along the intersection.

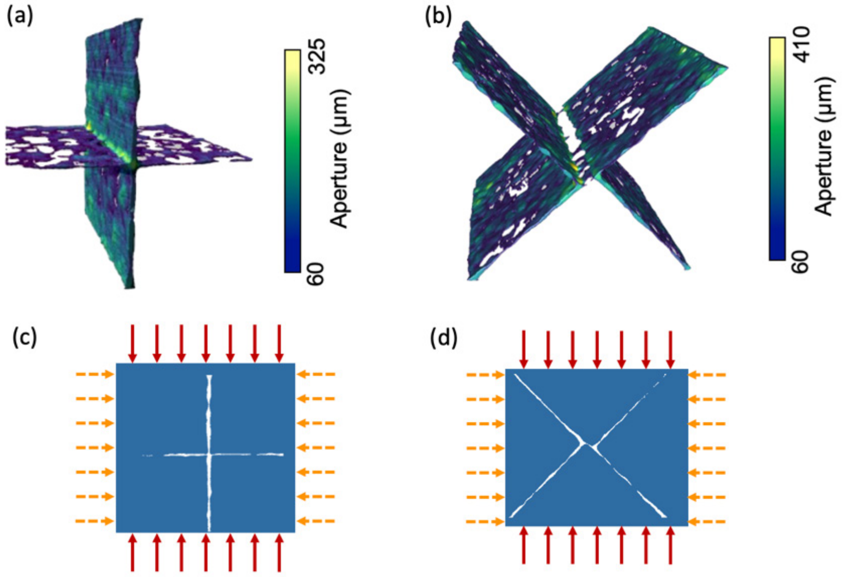

Figure 3. 3D X-ray tomographic reconstruction of aperture distribution for two different orientations (a) "+" and (b) "X" of a fracture network relative to the (c&d) applied stress (red arrows vertical load ~200 N & orange arrows weak confinement ~5N).

2.3 Pressure Solution—Coupled Geometry and THMC Processes at Interfaces

Pressure solution plays an important role in engineering and natural Earth systems where solid interfaces are often stressed while immersed in reactive fluids. Although not always widely recognized, pressure solution involves tight coupling between the geometry and THMC processes. These include (a) dissolution of minerals at interfaces that are subject to high contact stress, (b) diffusive transport of the dissolved species in the pore space, and (c) precipitation on relatively lower stressed crystal interfaces. As a result of pressure solution, the geometry of the solid surfaces and fluid chemistry are typically altered, leading to further changes in THMC processes in the subsurface.

In this section, recent work on modeling pressure solution is presented that rigorously considers the coupling of the evolving geometry and the THMC processes. First the compaction of a loosely packed salt aggregate (Hu et al. 2021) was simulated, and then the impacts of geometry and temperature on pressure solution in a natural salt rock were investigated (Hu et al. 2022).

Figure 4 shows the result of stress before pressure solution and porosity change due to pressure solution. Pressure solution preferentially dissolves sharp corners and edges that can lead to relatively high porosity loss in a system, and thus plays an important role in the creep of salt. Also, the dynamic changes of granular salt systems involve grain relocation and pressure solution can occur repeatedly and continuously during long-term creep behavior (Hu et al. 2021).

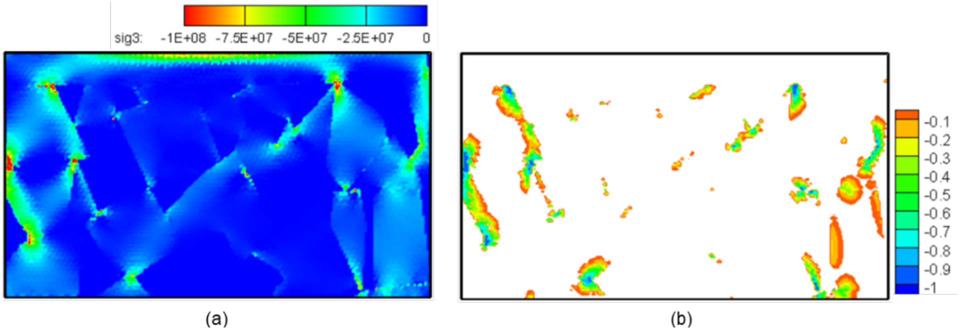

Figure 4. (a) Stress (Unit: Pa) before and (b) porosity change due to pressure solution (Hu et al. 2021).

In another example of natural salt rock, the results of scenarios are compared that only considered temperature (Case A, Figure 5b), only considered stress and no temperature (Case B) and considered both temperature and stress effects (Case C, Figure 5c). For Case A, temperature take effects on the individual pore space, which functions like isolated "islands" with dissolution at the hotter ends and precipitation at the cooler ends. By contrast for Case C, pressure solution removes the solid mass and connects these isolated pore spaces thus giving a larger space for diffusion and precipitation.

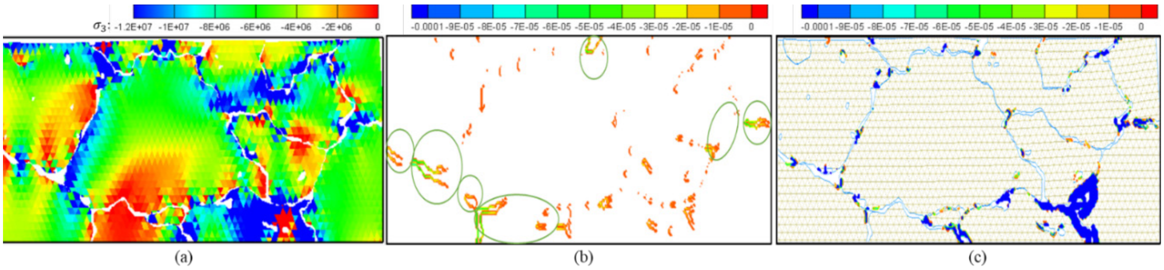

Figure 5. THMC modelling results of pressure solution in a natural salt rock: (a) Stress distribution (Unit: Pa), Dissolution rate (Unit: mol m-3 s-1) (b) only considering temperature and (c) considering pressure solution and temperature (Hu et al. 2022).

3 CONCLUSIONS

Earth systems consist of materials with complex geometric features undergoing complex coupled thermal-hydro-mechanical-chemical (THMC) processes. These geometric features when combined with THMC processes govern the formation and transformation of rocks and thus understanding their coupling is essential for rock engineering activities.

In this paper, we presented a series of numerical modeling and experimental results to address several scientific questions. Based on our simulations, we found that:

- Geometric features of fractures at different scales including asperities for single fractures and intersections for fracture networks are the key structural components that control the deformation of the fractures and fracture networks, thus affecting permeability at larger scales.
- Geometric features of grains at different scales including grain sharp corners (first-order geometric features) and roughness along grain boundaries (second-order geometric features) sequentially control compaction, stress distribution and pressure solution at different stages of sedimentation or mineral transformation (diagenesis, metamorphism).
- Depending on the stages of diagenesis (i.e., from grain aggregates to sedimentary rocks), first-order, second-order, and Nth-order geometric features sequentially play key roles in dominating contact dynamics, contact stress, and pressure solution in a sedimentary system

In summary, geometric features can be useful to detect the stages of sedimentation or mineral transformation (diagenesis, metamorphism) and to infer the changes of mechanical and flow properties that can be used as effective indices of the potential for energy recovery and storage.

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