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Authors
Rutqvist, Jonny
Birkholzer, Jens
Tsang, Chin-Fu

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Modelling Hydrological and Geomechanical Processes Related to CO₂ Injection in a Faulted Multilayer System

Jonny Rutqvist, Jens Birkholzer, Chin-Fu Tsang
Lawrence Berkeley National Laboratory,
Berkeley, CA 94720, USA

Abstract
This paper presents a numerical study of coupled hydrological and geomechanical processes during a deep underground injection of supercritical CO₂ in a hypothetical brine aquifer. We consider a multilayer system in which the injection zone is situated below a sequence of caprock and aquifer layers that are intersected by a vertical fault zone. The fault zone consists of highly fractured shale across the first caprock layers that are located just above the injection zone. Initially, the fractured shale zones are considered sealed with minerals, but we allow fractures (and the fractured zones) to open as a result of injection induced reductions in effective stresses. Our results indicate that even when assuming a very sensitive relationship between effective stress and fractured-zone permeability, the injection-induced changes in permeability across are only moderate with largest changes occurring in the first caprock layer, just above the injection zone. As a result, the upward leakage rate remains relatively small and therefore changes in fluid pressure and hydromechanical effects in overlying zones are also relatively small for the case studied in this paper.

Keywords: CO₂, storage, geomechanics, fault, leakage, hydromechanical

Introduction
Storage of CO₂ in deep brine formations has been suggested as one way to reduce greenhouse gases in the atmosphere. Trapping CO₂ at depth, underground requires a sufficiently impermeable caprock layer—or a sequence of such layers for increased safety and sequestration effectiveness—to prevent upward migration from the target reservoir. However, caprock layers may contain imperfections, such as faults or fracture zones, which can act as high-permeability conduits for leakage of CO₂ from depth to the near-surface environment. Further, hydraulic rock properties may be affected by increasing fluid pressure during injection. In this paper, we simulate the hydrological and geomechanical processes during and after injection of supercritical CO₂ into a deep brine formation. We consider a multilayer system, in which the injection reservoir is situated below a sequence of caprock and aquifer layers, which are intersected by a vertical fault (Figure 1). In Rutqvist et al. [1], we studied an equivalent system, in which the vertical fault was assumed to be highly permeable across the two lower caprocks, and we studied the potential for fracturing and shear failure within this system. We found that the upward migration of fluid pressure may cause significant changes in the stress field, and a relatively high potential for irreversible fault reactivation. In this paper, we consider a system in which the fault is initially sealed across the caprocks, but might be opened with changes as a result of the injection. We use a coupled reservoir-geomechanical simulation to evaluate the impact of such changes on the upward migration of CO₂.

Figure 1. Model geometry for simulation of CO₂ injection into a multilayered reservoir-caprock system
TOUGH-FLAC Simulator

The TOUGH-FLAC simulator [2] is based on coupling of two existing computer codes, TOUGH2 [3] and FLAC3D [4]. TOUGH2 is a well-established code for geohydrological analysis including multiphase, multicomponent fluid flow and heat transport, while FLAC3D is a widely used commercial code designed for rock and soil mechanics. For analysis of coupled thermal-hydrological-mechanical (THM) problems, the TOUGH2 and FLAC3D are executed on compatible numerical grids and linked through external coupling modules, which serve to pass relevant information between the field equations solved in the respective codes (Figure 2). A TOUGH-to-FLAC link takes multiphase pressures, saturation, and temperature from the TOUGH2 simulation and provides updated temperature, and pore-pressure information to FLAC3D (Figure 2). A FLAC-to-TOUGH link takes element stress and deformation from FLAC3D and updates element porosity, permeability, and capillary pressure to be used by TOUGH2. A TOUGH-FLAC coupling module for this link calculates the hydraulic property changes, based on material-specific theoretical or empirical functions.

Model Setup

In this application, the TOUGH2 part of the linked TOUGH-FLAC simulation includes the fluid property module ECO2N [5], which considers multiphase flow—in this case supercritical CO₂ and water—with dissolved or solid NaCl. The simulation was conducted in isothermal and linear elastic modes with material properties given in Table 1. The properties correspond to permeable sandstone layers with caprocks of shale as well as highly fractured shale where the fault line intersects the two lower caprocks. Permeability of the fractured shale is initially low, but still about 1 order of magnitude higher than the intact shale. An initially low permeability of the fractured shale may be envisioned such that a connected fracture network exists, but the fractures are initially sealed by minerals. In this application, the isotropic hydraulic properties are corrected using empirical porosity-mean stress and permeability-porosity relationships given in [6]. The parameters for the porosity-mean stress and permeability-porosity relationship for the intact host rock were estimated from laboratory data reported in the literature, which generally shows a one-order-of-magnitude reduction in permeability between zero and 30 MPa compressive effective stress [6]. For the highly fractured shale, the mean-stress-versus-permeability function is more sensitive than for intact rock, allowing stress-induced changes in permeability by several orders of magnitude.

Transient numerical simulations with TOUGH-FLAC are conducted for a time period of 500 years, with injection of CO₂ occurring over the first 30 years.
Results
To evaluate the impact of pressure-induced changes in hydrological properties, we first compare simulations with and without consideration of hydromechanical couplings. Figure 3 shows the distribution (in the form of saturation values) of the CO₂-rich phase (supercritical CO₂ with small amounts of dissolved water) at the end of the 30-year injection phase, and after 500 years (i.e., 470 years after the end of the injection phase). The result shows that when hydromechanical coupling is considered, the permeability in the fractured shale zones across caprocks 1 and 2 have increased sufficiently to allow increased upward leakage of CO₂. After 30 years, the CO₂ has penetrated two layers of caprock when hydromechanical coupling is considered. At 500 years, the CO₂-plume in the upper aquifer has widened and increased in size, demonstrating that buoyancy forces continue to enforce upward flow of CO₂ through the fracture zones long after injection has ceased.

Figure 4 presents the time-evolution of fluid pressure, changes in fracture zone permeability, and CO₂ flux and cumulative CO₂ mass through the fractured zones across caprocks 1 and 2. Figure 4b shows that the pressure-induced changes in fracture zone permeability first occurs in Caprock 1, immediately above the injection zone, and thereafter continues upwards as increasing fluid pressure propagates upward. A maximum permeability change of about 1 to 2 orders of magnitude occurs near the lower part of Caprock 1, where the pressure increase is the highest. However, the simulation results indicate that the fluid pressure only increases very slowly in the overlying zones 2 and 3, and therefore pressure-induced changes of permeability in upper parts of Caprock 1 as well as Caprock 2 are relatively small and delayed in time. Nevertheless, the pressure-induced permeability changes cause leakage to occur across Caprock 1 after about 10 years and (later) across Caprock 2 after about 30 years. However, the total mass that leaked into the overlying zones is only few percent of the injected CO₂ mass, even after 500 years (Figure 4d). Moreover, because the leakage rates are relatively small across Caprock 1, and the fluid pressure does not change as much in the overlying zones or in caprocks 2 and 3. This finding demonstrates the benefits of a layered system, in which high-permeability zones overlay the caprock layers—not only as a hydrodynamic trap, but also to attenuate fluid pressures in the upper parts of the system, thereby reducing the overall hydromechanical changes in the system.

We also analyze the potential for a rock-mass mechanical failure by evaluating (1) the critical pressure that could induce hydraulic fracturing or (2) the critical pressure that could induce shear slip along pre-existing fractures (see [1] and [6] for details on the shear-slip analysis model). We use the conservative assumption that a hydraulic fracture could develop as soon as the fluid pressure exceeds the least compressive principal stress. We also use the conservative assumption for the onset of shear slip that a pre-existing fracture could exist at any point with an arbitrary orientation. In this simulation, we test the potential for shear slip assuming zero cohesion and a friction angle of 30°.

Figure 5 presents distribution of changes in fluid pressure and mean effective stress, which are important factors in evaluating system hydromechanical changes. Figure 5a shows that at 30 years, the fluid pressure has increased (by 10 MPa) to 26 MPa in the injection zone, which is well below the lithostatic stress. (The lithostatic stress is about 35 MPa at the injection level, based on the weight of the overlying rock mass.) In Figure 5b, changes in mean effective stress ($\Delta\sigma'_m = [\Delta\sigma'_x+\Delta\sigma'_y+\Delta\sigma'_z]/3$) are shown. In general, the mean effective stress decreases with the increasing fluid pressure in the injection zone, with a stress change about 60% of the change in fluid pressure. The reduction in effective stress with fluid pressure is counteracted by horizontal poro-elastic stressing that increases the confining stresses in the horizontal direction.

Figure 6 presents the potential for fault slip for two different anisotropic stress regimes—an extensional stress regime and a compressional stress regime (little or no potential for fracturing occurred and is not shown). The results in Figure 6 are presented in terms of pressure margins to onset of shear slip [1, 6].
A positive pressure margin would imply that the local fluid pressure is above the critical pressure for onset of hydraulic fracturing of shear slip, and hence dark contours would indicate areas of the highest damage potential. Figure 6 shows that the highest potential for onset of shear occurs within the injection zone and in the lower parts of Caprock 1, in the case of a compressional stress regime (Figure 6a). For the extensional stress regime, on the other hand, the highest potential for onset of shear occurs in the overburden rock and within the fracture zone (Figure 6b). However, the pressure margin is negative in the entire model, indicating that fluid pressure is below the critical pressure, and no shear would take place.

The results in Figure 6 indicate much less potential for shear slip than reported in Rutqvist et al. [1]. In Rutqvist et al. [1], the fault zones were assumed to be initially open and highly permeable, and thus fluid pressure could rapidly propagate into the overlying zones. On the other hand, in the study presented in this paper, the permeability of the fault zones does not increase enough for a significant upward leakage and change in fluid pressure in the overlying formations. As a result, significant changes in effective stress are confined within and near the injection zone, and the potential for shear slip in the upper parts of the multilayer system is much reduced.

Conclusions
Our results demonstrate that CO₂ sequestration below multilayer geological system of high and low (caprock) permeability layers, is beneficial for reducing the risk for damaging geomechanical effect in the system. Potentially damaging changes in fluid pressure in the upper parts the multi-layered system can only occur if the caprocks are discontinuous or are intersected by highly permeable fault zones. If a fault zone exist, but is initially sealed across the caprocks, some pressure-induced changes in permeability could occur, especially just above the injection zone. However, even when assuming a very sensitive relationship between effective stress and fractured-zone permeability, the injection-induced changes in permeability are only moderate. As a result, the upward leakage rate remains relatively small and therefore changes in fluid pressure and hydromechanical effects in overlying zones are also relatively small for the case studied in this paper. Thus, hydromechanical changes and potential for damage are much less likely for a system where substantial upward migration of fluid pressure can be prevented.

Figure 3. Distribution of CO₂-rich phase at 30 years (end of injection) and 500 years with and without consideration of fluid-pressure-induced changes in permeability
Acknowledgment
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References

Figure 4. Time evolution of (a) fluid pressure, (b) permeability change factor, (c) upward CO2 fault leakage, and (d) leaked CO2 mass relative to injected CO2 mass
Table 1. Material Properties

<table>
<thead>
<tr>
<th>Property</th>
<th>Injection Zone</th>
<th>Caprock</th>
<th>Overlying Zones</th>
<th>Fault Zone (10 m wide)</th>
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<tr>
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</table>

Figure 5. Changes in (a) fluid pressure, and (b) effective mean stress after 30 years of injection

Figure 6. Contours of pressure margin ($P_{sm} = P - P_{critical}$) for shear slip in the case of (a) a compressional stress regime in which $\sigma_H = 1.5 \sigma_V$ and an (b) extensional stress regime in which $\sigma_H = 0.7 \sigma_V$