Three-Dimensional Modeling of the Reactive Transport of CO₂ and Its Impact on Geomechanical Properties of Reservoir Rocks and Seals

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Abstract: This article develops a model to analyze CO₂ reservoirs using the STOMP-CO2-R code that is interfaced with the ABAQUS[®] finite element package. The STOMP-CO2-R/ABAQUS[®] simulator accounts for the reactive transport of CO₂ causing **changes in mineralogy** that modify the geomechanical properties of reservoir rocks and seals. Rocks' elastic properties that vary during CO₂ injection and govern the poroelastic behavior of rocks are modeled by an Eshelby-Mori-Tanka approach. A three-dimensional (3D) STOMP-CO2-R model for a CO₂ reservoir containing a vertical fault **was** built to analyze a formation containing a reaction network with 5 minerals: albite, anorthite, calcite, kaolinite and quartz. A 3D ABAQUS[®] model that maps this STOMP-CO2-R model **was** built for the analysis using STOMP-CO2-R/ABAQUS[®]. The results show that after a long period of CO₂ injection the mineralogical changes significantly reduced the permeability and elastic modulus of the reservoir in front of the fault leading to a reduction of the pressure margin to fracture at and beyond the injection location. The impact of reactive transport of CO₂ on the geomechanical properties of reservoir rocks and seals are studied in terms of mineral composition changes that affect the rock stiffness, stress and strain distributions, and pressure margin to fracture.

Keywords: CO₂ reservoir; reactive transport; geochemistry; geomechanics; geomechanical modeling; mineral composition; homogenization; fault; hydraulic fracture; elastic modulus

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1. Introduction

The description of a session on “*Coupled hydraulic, geochemical, and geomechanical processes in carbon storage*” at the 2014 AGU Fall Meeting stated: “Safe long-term storage of CO₂ in the subsurface requires a detailed understanding of several distinct but interdependent processes: (i) flow and transport of CO₂ and brine; (ii) thermal effects of injection; (iii) CO₂-induced chemical reactions; and (iv) mechanical impacts of injection on the reservoir, caprock and the wellbore.” **There have been significant studies on separated processes or the couplings between flow and geomechanical, or flow and geochemical processes.** For instance, the impact of gas injection on the induced geomechanical effects has been addressed (Ferronato et al., 2010; Preisig and Prévost, 2011; Streit and Hillis, 2004; Teatini et al., 2014). Important geomechanical processes may take place depending on the injection scenarios/design and site conditions for either CO₂ sequestration, CH₄ storage, or enhanced oil recovery in real geologic settings (Chiaramonte et al., 2008; Fokker et al., 2011; Rutqvist, 2012; Rutqvist et al., 2010; Teatini et al., 2011; Verdon et al., 2011; Vidal-Gilbert et al., 2010; Vidal et al., 2002). These above studies utilized coupled hydraulic and geomechanics modeling, without considering geochemical processes.

In parallel, there has also been a significant amount of work on coupling hydraulic and geochemical processes (André et al., 2007; Audigane et al., 2007; Johnson et al., 2004; Nghiem et al., 2004; Noh et al., 2007; Pruess et al., 2003; Xu et al., 2006). However, to date, little work has been reported on fully coupling flows to both geochemical and geomechanical processes. The pioneering work by (Bissell et al., 2011; Johnson et al., 2004; Johnson et al., 2005; Kvamme and Liu, 2009; Rutqvist et al., 2014) are promising. Bissell et al. (Bissell et al., 2011) coupled geomechanical calculations to fluid flow with an energy transport equation and simulated two-phase immiscible flow with four components (CH₄, CO₂, NaCl and H₂O) in the gas and aqueous phases in a saline aquifer. Johnson et al. (Johnson et al., 2004; Johnson et al., 2005) introduced a coupled modeling framework that evaluates geochemical counterbalancing of geomechanical aperture evolution as a function of effective diffusion distance and reaction progress. Their studies suggested that ultimate counterbalancing of geochemical and geomechanical effects is feasible, and, therefore, that shale caprocks may in fact evolve into effective seals—in both natural and engineered storage sites. Kvamme and Liu (Kvamme and Liu, 2009) developed a reservoir simulator for the thermo-hydro-mechanical analysis of multiphase saline media, and demonstrated the approach using a two-dimensional (2D) hydro-chemical-mechanical problem. Rutqvist et al. (Rutqvist et al., 2014) conducted simulation of coupled thermal, hydrogeological, mechanical, and chemical (THMC) processes in the engineered barrier system and near-field rock associated with high-level radioactive waste repositories hosted in clay formations. The above studies considered fluid flow, reactive transport, and geomechanical process, but they were generally performed within 2D modeling domains due to computational complexity and demand. Also, mechanics models to capture the evolving mineral compositions and translate them in geomechanical properties were absent.

Although 2D models are practical and helpful to analyze coupled processes, they are not able to fully represent a geological formation with all its complexities, so they cannot accurately capture the stress and strain distributions resulting from the interactions between the various processes that are discussed above and govern CO₂ injection and storage (Moretti et al., 2006; Orlic et al., 2001; Zheng et al., 2009). This paper addresses coupled hydrological, geochemical and geomechanical processes through three-dimensional (3D) numerical simulations. The thermal effects of injection have been addressed elsewhere (Bonneville et al., 2014; Goodarzi et al., 2012; Gor et al., 2013; Lu and Connell, 2008) and can be included in modeling the hydro-geochemical-mechanical processes in our future work. CO₂-induced chemical reactions can significantly modify the geomechanical behavior of rocks, since CO₂ can react with the constituent phases of reservoir rocks and modify their compositions. This can lead to modifications of their permeability and geomechanical properties including poroelastic properties, stress/strain behavior, and strength. Modifications of rock geomechanical properties have important consequences as these directly control stress and strain distributions, and affect conditions for fracture initiation and propagation. Long-term caprock integrity is the most important requirement for CO₂ storage sites. Geochemical alterations of the rock composition can enhance or degrade the seal integrity depending on the governing chemical reactions with CO₂. In parallel, precipitation or dissolution of minerals can heal or weaken a fault as the stiffness and strength of the fault zone can be increased or degraded.

In this paper, we develop and demonstrate a 3D modeling capability with fully coupled flow, geochemistry and geomechanics to realistically model the reactive transport of CO₂ and its impact on geomechanical properties of faulted reservoir rocks and seals. This capability has been achieved by sequentially coupling Pacific Northwest National Laboratory's code named STOMP-CO₂-R (White et al., 2012; White and McGrail, 2005) to the commercial ABAQUS[®] finite element package. The STOMP-CO₂-R/ABAQUS[®] sequentially coupled simulator accounts for the reactive transport of CO₂ causing mineral composition changes that modify the geomechanical properties of reservoir rocks and seals. Formation rocks' elastic properties that vary during CO₂ injection and govern the poroelastic behavior of rocks are modeled by an Eshelby-Mori-Tanka approach (EMTA) implemented in ABAQUS[®] via user-subroutines. The computational tool accounts for the change in rock permeability due to both geochemistry and geomechanics. A STOMP-CO₂-R model for a model CO₂ reservoir containing a vertical fault was built for the reservoir analysis. A simplified geochemical reaction network with 5 minerals was considered: albite, anorthite, calcite, kaolinite and quartz (Fischer et al., 2013; Tremosa et al., 2014; Yang et al., 2014). The reservoir consists mainly of quartz with lesser amounts of albite and anorthite; the caprock consists largely of kaolinite and quartz. An ABAQUS[®] model that maps the above STOMP-CO₂-R model for the formation was built for the sequentially coupled analysis using STOMP-CO₂-R/ABAQUS[®]. We have developed this model to demonstrate that coupled geochemistry and geomechanics can have significant impacts on CO₂ injection and reservoir properties with reactive minerals. We assumed the target reservoir was a

feldspathic arenite with anorthite that dissolves relatively rapidly as pH is lowered. This composition was inspired by the presence of reactive anorthite in samples from the Ketzin Site (Fischer et al., 2013).

The modeling feature in this work is summarized as follows. At the molecular and phase scale, geochemical modeling handles the evolution of mineral volume fractions that feeds into the EMTA micromechanics to compute the elastic properties of reservoir rocks. These properties are then used as material properties inputs for different layers of a geological site (macroscopic geological scale). It is noted that these scales are not treated independently, but a lower scale is bridged to an upper scale.

2. Multiphase flow and reactive transport model

This section describes the chemical reactions and the models to capture the evolution of mineral composition related to the reactive transport of CO₂ in reservoirs. It also presents of the models used in the analysis of flow in porous media.

2.1 Chemical reactions and mineral composition evolution

The chemical reactions caused by CO₂ injection begin with the dissolution of CO₂ in water to form weak carbonic acid:

This is followed by dissociation of carbonic acid to form the bicarbonate ion:

The increased acidity causes dissolution of primary host rock minerals, which in turn causes complexing of dissolved cations with the bicarbonate ion. The dissolved bicarbonate species react with divalent cations to precipitate carbonates. Formation of carbonates is expected to be the primary mechanism by which CO₂ is mineralized (Gunter et al., 1997). CO₂ solubility in brine is computed using the Battistelli-et-al. formulation (Battistelli et al., 1997) as a function of temperature and salt molality.

Mineral precipitation and dissolution are assumed to be described by the transition state theory based on which the rate equation (Lasaga, 1984; Steefel and Lasaga, 1994) is expressed as

$$R_r = A_m r \left[1 - \frac{Q}{K_{eq}} \right] \quad (3)$$

where ‘m’ is the mineral index, R_r is the dissolution or precipitation rate (positive values indicate dissolution, and negative values precipitation), A_m is the specific reactive surface area, parameter r is the rate constant (moles per unit mineral surface area and unit time) which is temperature dependent, K_{eq} is the equilibrium constant for the mineral-water reaction written for the destruction of one mole of mineral ‘m’, and Q is ion activity product. The temperature dependence of the reaction rate constant can be expressed reasonably well via an Arrhenius equation (Lasaga, 1984; Steefel and Lasaga, 1994). Since many rate constants are reported at 25°C, it is convenient to approximate the rate constant dependency as a function of temperature,

$$r = r_{25} \exp \left[\frac{-E_a}{R} \left(\frac{1}{T} - \frac{1}{298.15} \right) \right] \quad (4)$$

where E_a is the activation energy, r_{25} is the rate constant at 25°C, R is gas constant, and T is absolute temperature. Activity coefficients for aqueous species are calculated using the B-dot formulation of Helgeson (1969).

The domain of the model reservoir analyzed in this paper contains two rock types that are simplified versions of sandstone and shale. The sandstone has 12% porosity, and the shale 5.1%. The mineral composition for each rock type, with dissolution and precipitation rate parameters for each mineral (Palandri and Kharaka, 2004; Xu et al., 2007), is given in Table 1.

The equilibrium constant K_{eq} is assumed to be a nonlinear function of temperature

$$\log K_{eq} = a \ln T + b + cT + \frac{d}{T} + \frac{e}{T^2} \quad (5)$$

where T is temperature in Kelvin, and a , b , c , d and e are the equilibrium constant temperature coefficients. Table 2 lists the kinetic reactions and these coefficients in Equation (5) for the minerals while Table 3 gives the aqueous equilibrium reactions and these coefficients (a , b , ..., e) for the aqueous phase.

As the minerals dissolve and precipitate, porosity changes are related to the change in the molar density of each mineral by the mineral density and molecular weight

$$d\phi = \frac{dm}{\rho_g} M_w \quad (6)$$

where m denotes the molar density (moles per volume) of mineral, ϕ is the porosity, M_w , molecular weight of mineral, and ρ_g , mineral density. Table 4 provides the mineral density and molecular weight for each mineral listed in Table 1.

The model proposed by (Verma and Pruess, 1988) was used to relate changes in porosity with changes in intrinsic permeability:

$$\frac{k}{k_0} = \left(\frac{\phi - \phi_0}{\phi_0 - \phi_c} \right)^n \quad (7)$$

where k_0 , k , ϕ and n are the initial and current intrinsic permeability, porosity and power-law exponent (e.g., $n = 2$ in this study), respectively. The critical porosity ϕ_c is defined as 80% of the initial porosity ϕ_0 .

2.2 STOMP-CO2-R analysis of flow in porous media

The multiphase mass conservation equation is

$$\frac{\partial}{\partial t} \left[\sum_{\gamma=l,g,p} (\phi \rho_\gamma s_\gamma u_\gamma) \right] = - \sum_{\gamma=l,g} \nabla (\rho_\gamma h_\gamma \mathbf{V}_\gamma) + \nabla (\mathbf{k}_e \nabla T) + \sum_{\gamma=l,g} \nabla (h_\gamma m_\gamma) + q \quad (8)$$

where $\gamma = l, g, p$ represents liquid, gas, and salt respectively. ϕ , ρ , s , and u denote porosity, density, saturation, and velocity respectively. h , $\mathbf{V}$, $\mathbf{k}_e$, T , m , q are the head, advective flux, effective thermal conductivity, temperature, mass rate density, and volumetric flow rate, respectively.

The saturation–capillary pressure relations are described by (Brooks and Corey, 1966). When CO₂ is injected into a deep saline geologic reservoir, initially the aqueous phase is displaced. As injection continues, the aqueous relative permeability drops, especially near the injection point, and the formation rock begins to desaturate through desiccation by the injected CO₂. Conventional capillary pressure and saturation functions are limited to saturations above the residual saturation. For these functions, the capillary pressure tends toward infinity as the aqueous saturation approaches the residual saturation. This limitation can be overcome by specifying an extension option, for example, the Webb (Webb, 2000) extension divides the capillary pressure-saturation function into two regimes. For low aqueous saturation the function follows a logarithmic form, and for moderate to high saturations the function follows the specified form (e.g., (Brooks and Corey, 1966)).

For the aqueous and gas relative permeability functions, a number of functional forms are available. We adopted the Burdine model (Burdine, 1953) model where aqueous relative permeability depends on the effective aqueous saturation and porosity distribution factor, while gas relative permeability depends on the effective free gas saturation, apparent aqueous saturation, and porosity distribution factor. The saturation functions and the aqueous and gas relative permeability functions use the Burdine pore-size distribution model are shown in Equations (9-13).

$$\bar{s}_l = \begin{cases} \left(\frac{P_g - P_l}{\bar{\rho}_l g} \right)^{-\lambda} & \text{for } (P_g - P_l) \geq P_0, \\ \bar{s}_l = 1 & \text{for } (P_g - P_l) < P_0 \end{cases} \quad (9)$$

$$s_l = \bar{s}_l(1 - \bar{s}_m) + \bar{s}_m, \quad (10)$$

$$\bar{s}_g = 1 - \bar{s}_l, \quad (11)$$

$$k_{rl} = (\bar{s}_l)^{3+2/\lambda}, \quad (12)$$

$$k_{rg} = (\bar{s}_g)^2 [1 - (\bar{s}_l)^{1+2/\lambda}], \quad (13)$$

where P_g is the gas pressure, P_l the aqueous pressure, $\bar{s}_l$ the effective aqueous saturation, S_l the actual aqueous saturation, $\bar{\rho}_l$ is reference aqueous density, P_0 the Brooks and Corey air-entry pressure (in meters), $\bar{s}_m$ the effective residual aqueous saturation, λ the Brooks and Corey fitting parameter, $\bar{s}_g$ the effective aqueous saturation, k_{rl} the aqueous relative permeability, and k_{rg} the gas relative permeability. The major hydrogeological parameters, such as hydrological function parameters for Brooks-Corey and Burdine models, were measured or inferred along some characterization wells near the reference site from the Mount Simon formation, and are summarized in Table 5.

The pure-water liquid viscosity is computed as a function of temperature, pressure, and density using ASME steam table formulations (Meyer, 1993). Brine viscosity is computed from the pure-water liquid viscosity as a function of salt molality and temperature using the formulation of Phillips et al (1981). Aqueous viscosity is computed from the brine viscosity, pure CO₂ viscosity, and aqueous-CO₂ mole fraction, using the formulation of Grunberg and Nissan (Reid et al., 1987). Gas viscosity is computed from the pure component viscosities of CO₂ and water vapor using an extension proposed by Wilke of the Chapman-Enskog theory for multi-component gas mixtures at low densities (Reid et al., 1987). The semi-empirical expression of Wilke relates the gas mixture viscosity to the pure component vapor viscosities and component gas mole fractions.

The flow and reactive transport processes are simulated simultaneously at each simulation step, by solving the multiphase flow and reaction transport equations, where the reactive transport is simulated by the module named “EKEChem”.

3. Geomechanical model

3.1 Eshelby-Mori-Tanaka approach to geomechanics

There is a large body of literature on micromechanical models addressing the prediction of elastic properties of composite materials containing fibers, particles or more generally inclusions embedded in a matrix phase. In particular, there is a family of models that has evolved from a proposal initially made by (Mori and Tanaka, 1973). To date, the Eshelby's equivalent inclusion method (Eshelby, 1957) combined with a Mori-Tanaka type model (Benveniste, 1987) presents one of the most efficient and accurate methods for the prediction of elastic properties of the homogenized composite from features and elastic properties of the constituents. The constituent features are their shapes and distributions in the matrix materials. The Eshelby-Mori-Tanka approach (EMTA) was previously used by Guéry et al. (Guéry et al., 2010) to compute the elastic stiffness of an argillite rock modeled as three-phase composite. These authors found that the EMTA model was able to correctly reproduce the experimental data. At the best of the authors' knowledge the EMTA models have not been used in the context of 3D modeling of CO₂ reservoir sites that involve reactive transport of CO₂ modifying the rock mineral compositions. Our preliminary work on this subject can be found in (Nguyen et al., 2014). The expression of the stiffness tensor for an m -aligned-inclusion-phase composite according to the EMTA is

$$\mathbf{C} = \mathbf{C}_0 + \sum_{i=1}^m v_i (\mathbf{C}_i - \mathbf{C}_0) \mathbf{A}_i \quad (14)$$

where $\mathbf{C}_i$ and $\mathbf{C}_0$ are the elastic stiffness tensors of inclusion i and of the matrix material, respectively. v_i denotes the inclusion Poisson's ratio, and $\mathbf{A}_i$ are the inclusion strain concentration tensor given by

$$\mathbf{A}_i = \mathbf{T}_i \left[v_0 \mathbf{I} + \sum_{i=1}^m v_i \mathbf{T}_i \right]^{-1} \quad (15)$$

with $\mathbf{I}$ being the identity tensor, v_0 the matrix Poisson's ratio, and $\mathbf{T}_i$ given by:

$$\mathbf{T}_i = [\mathbf{I} + \mathbf{S}_i \mathbf{C}_0^{-1} (\mathbf{C}_i - \mathbf{C}_0)]^{-1} \quad (16)$$

where $\mathbf{S}_i$ is the Eshelby tensor of inclusion i that depends on the inclusion aspect ratio and the matrix elastic properties. Expressions of $\mathbf{S}_i$ for different inclusion shapes are given by (Mura, 1987). Following is the expression of the Eshelby tensor in index notation for spherical elastic inclusions:

$$S_{ijkl} = \frac{5\nu_0 - 1}{15(1 - \nu_0)} \delta_{ij} \delta_{kl} + \frac{4 - 5\nu_0}{15(1 - \nu_0)} (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}) \quad (17)$$

where δ_{ij} is the Kronecker delta, $\delta_{ij} = \begin{cases} 0 & \text{if } i \neq j \\ 1 & \text{if } i = j \end{cases}$.

The formation rock materials considered in this paper contain four solid inclusion phases which are albite, calcite, kaolinite, and anorthite in addition to pores that are embedded in the

quartz matrix. For the sake of simplicity but still keeping track of the important presence of each phase, we assume that all the inclusions including pores have spherical shapes as schematically depicted in **Figure 1**. In addition, the pores are modeled as inclusions with infinitesimal elastic modulus, and all the phases are uniformly and randomly distributed in the quartz matrix. Numerically, it is necessary to assign a very small but nonzero value of the elastic modulus for the pores ($\sim 10^{-8}$ MPa). The stiffness of such a homogenized rock material is computed by **Equation (10)** with $m = 5$. The uniform and random distributions of inclusions render the behavior of homogenized rocks isotropic.

EMTA performs a rigorous homogenization to achieve the homogenized elastic properties of rocks that are used as material property inputs for the formation layers described in the paper. Such a homogenization procedure is very powerful and efficient in that it accurately computes the homogenized elastic properties for a rock material (mesoscale) based on its composition and features of the constituents (microscale), and in the meantime, keeps track of the information of the microscale (e.g., evolving mineral volume fraction). The evolution of mineral volume fractions predicted by STOMP-CO2-R is captured by EMTA to compute the resulting rock elastic properties. Without EMTA or an equivalent micromechanical model, there is no way to accurately determine the rock elastic properties from elastic properties of the mineral constituents.

3.2 Poroelastic constitutive relations

The poroelastic constitutive equations in the principal stress axes system are given by

$$\sigma_{ij} = C_{ijkl} \varepsilon_{kl} - \alpha_{ij} P \quad (18)$$

where C_{ijkl} are the stiffness tensor of the homogenized rock material without fluid, i, j, k , and l are the indices denoting the tensor components, σ_{ij} and ε_{ij} are mechanical stress and total strain tensors, respectively. **Tensile stresses are positive**. Einstein's notations for the index variables are used in **Equation (18)**. C_{ijkl} is computed using **Equation (14)** accounting for the rock mineral composition. α_{ij} denotes the Biot's tensor. For an isotropic rock, $\alpha_{11} = \alpha_{22} = \alpha_{33}$ and $\alpha_{ij} = 0$ with $i \neq j$. In this work, we consider $\alpha_{11} = \alpha_{22} = \alpha_{33} = 1$ for all rock materials. P is the pore fluid pressure that is determined in terms of aqueous and gas pressures, P_a and P_g as well as aqueous and gas saturations, S_a and S_b as (Rutqvist and Tsang, 2002):

$$P = S_a P_a + (1 - S_a) P_g \quad (19)$$

The pore fluid pressure is the saturation-weighted sum of the partial pressures of the individual fluid phases.

The porosity is computed in terms of the volumetric strain, ε_v as (Cappa and Rutqvist, 2011; Chin et al., 2000)

$$\phi = 1 - (1 - \phi_0) e^{-\varepsilon_v} \quad (20)$$

with $\varepsilon_v = \varepsilon_{ii} = \varepsilon_{11} + \varepsilon_{22} + \varepsilon_{33}$ being the volumetric strain.

From Equation (18), the effective principal stresses are computed as:

$$\sigma'_{ij} = \sigma_{ij} + \alpha_{ij} P = C_{ijkl} \varepsilon_{kl} \quad (21)$$

The principal effective stresses also determine the Mohr-Coulomb fracture criterion (Jaeger and Cook, 1979) according to which assuming zero-tensile strength, hydraulic fracture could develop as soon as the fluid pressure exceeds the least compressive principal stress. In other words, all the principal effective stress components should be negative to avoid hydraulic fracture, and as soon as a component becomes or exceeds zero, hydraulic fracture is predicted to occur. As a consequence, the least compressive principal stress defines the *pressure margin to fracture* (PMF):

$$PMF = \text{Max}(\sigma'_{11}, \sigma'_{22}, \sigma'_{33}) \quad (22)$$

The tendency to slip is predicted using the Mohr-Coulomb criterion (Jaeger and Cook, 1979):

$$\tau = c_0 + \mu_s \sigma'_n \quad (23)$$

where τ is the critical shear stress for slip occurrence, σ'_n denotes the effective normal stress on the fault plane, and c_0 and μ_s are the cohesion and static friction coefficients, respectively. For a well-established and cohesionless fault, $c_0 = 0$ (Streit and Hillis, 2004), slip occurs if the slip tendency factor on the fault plan is equal to or exceeds μ_s :

$$\frac{\tau}{\sigma'_n} \geq \mu_s \quad (24)$$

μ_s is defined in terms of the friction angle φ as $\mu_s = \tan(\varphi)$. Our approach using the Mohr-Coulomb failure criterion to predict the occurrence of hydraulic fracture and shear failure by slip is a conservative approach assuming zero tensile strength and cohesionless fault. It does not model any progressive damage and failure mechanisms leading to mechanical failure for the scenario investigated or other possible scenarios. A model for rock damage and fracture that impact rock permeability can be incorporated in the current modeling framework and will be developed in our future work. Table 7 provides the values of the parameters used in the failure criteria.

Figure 1. Schematic of the mineral composition for the formation rocks considered in the EMTA homogenization (Nguyen et al., 2015).

4. Coupled model interface and computational procedure

The geochemical-mechanical analysis of a model CO₂ reservoir discussed in the following sections was performed using PNNL's STOMP-CO₂-R code that has been interfaced with the commercial ABAQUS[®] finite element package. The poroelastic constitutive relations including the EMTA model for 5 inclusion phases in the quartz matrix have been implemented in ABAQUS[®] using user subroutines. The STOMP-CO₂-R/ABAQUS[®] coupled analysis is executed sequentially in series. This means that for a given period of analysis the exchange data between STOMP-CO₂-R and ABAQUS[®] occurs at the selected times prescribed in advance, and a STOMP-CO₂-R execution is followed by an ABAQUS[®] execution, and so on. A program written in Python was developed to control the serial executions and the exchange of output data between these codes. **Figure 2** provides the structure of the STOMP-CO₂-R/ABAQUS[®] simulator. For the analysis of a geological formation, a STOMP-CO₂-R model of the formation is built to perform the simulation of flow and reactive transport of CO₂ in the formation that is a complex multilayer system containing a CO₂ reservoir comprised between basement and caprock. The formation can contain faults crossing through different layers. An ABAQUS[®] finite element model of the same formation is built that exactly maps the STOMP-CO₂-R grid allowing the exchange of data between STOMP-CO₂-R and ABAQUS[®]. At selected times, STOMP-CO₂-R provides ABAQUS[®] with the coordinates, aqueous pressure and saturation, gas pressure and saturation, and volume fractions of constituent phases including porosity as well as

the intrinsic permeability at each STOMP-CO2-R cell center. Those cell centers are also ABAQUS[®] finite element centroids. Using STOMP-CO2-R results as input, ABAQUS[®] computes the element stiffness using the EMTA model and integrates the poroelastic constitutive relations according to Equations (18) to (21). Specifically, the stiffness matrix $\mathbf{C}$ (or C_{ijkl} in index notation) computed by the EMT approach (Equation(14)) based on mineral volume fractions determined by STOMP-CO2-R is used in the poroelastic constitutive relation (Equation (18)) to compute the total stress tensor as a function of the total strain tensor. Next, the volumetric strain ε_v is computed to update the porosity based on geomechanics using Equation (20). The updated porosity is then provided to STOMP-CO2-R to proceed to the next time step. The capillary entry pressure is computed in terms of the entry pressure, permeability and porosity based on a relation by (Leverett, 1941) also used by (Rutqvist and Tsang, 2002): $P_c = P_0 \sqrt{k_0 / \phi_0} / \sqrt{k / \phi}$, where P_0 is the zero stress initial entry pressure, and was chosen based on Mount Simon survey information. After updating the stresses, the pressure margin to fracture is computed by Equation (22). Assuming zero-tensile strength, hydraulic fracture is predicted to occur if the pressure margin to fracture is equal to or exceeds zero. This fracture criterion is applied to all the integration points of the modeling domain including basement, reservoir and caprock. In the model, the fault extends from the bottom of the basement to the top surface of the caprock. Finally, the slip tendency factor for an element on a fault segment is calculated using Equation (24). The change in permeability in the formation including the fault is governed by the change in porosity due to both geochemistry and geomechanics according to Equations (6), (7) and (20). The permeability change affects the fluid pressure which in turn affects the effective normal stress on the fault plane in the calculation of the slip tendency factor by Equation (24). The model does not compute changes in permeability for elements that have mechanically failed. At each selected time, ABAQUS[®] provides STOMP-CO2-R with the updated capillary pressure, porosity based on Equations (19-20), and updated quartz volume fraction. As the pores are modeled in the EMTA mechanics as inclusions embedded in the quartz matrix, the change in porosity under the geomechanical action leads to a corresponding change in the quartz volume fraction accordingly. The coupling between geochemistry and geomechanics is explicitly conducted through Equations (7) and (20) as well as the Leverett equation giving the capillary entry pressure in terms of the permeability and porosity.

Figure 2. STOMP-CO2-R/ABAQUS computational procedure (Nguyen et al., 2015).

PNNL's STOMP-CO2 version for analysis of multiphase flows in porous media without chemical reactions has also been interfaced with ABAQUS® in a similar procedure to the one depicted in **Figure 2** for STOMP-CO2-R/ABAQUS® except there are no chemical reactions considered, and therefore, the geomechanical properties for each rock material are constant. In the Results and Discussion section comparative analyses of a model reservoir using STOMP-CO2/ABAQUS® and STOMP-CO2-R/ABAQUS® will be presented to discuss the geochemical and geomechanical effects.

5. Model domain

5.1 STOMP-CO2-R 3D model

This section describes a STOMP-CO2-R 3D model reservoir used to study the effects of the reactive transport of CO₂ on geomechanical properties of reservoir rocks and seal using the STOMP-CO2-R/ABAQUS® simulator. The formation was discretized into $27 \times 20 \times 37$ grid cells. The CO₂ injection point is 3000 meters (m) away from the horizontal boundaries. The formation domain depicted in **Figure 3** consists of three layers: caprock, reservoir, and basement. The bottom elevation of the formation is assumed to be 1800 m below the ground surface. A vertical fault is assumed to penetrate through the three layers parallel to the y-axis (i.e., along the

north-south direction) and located 1200 m away from the injection point. The injection zone extends from the bottom of the reservoir to the reservoir/caprock interface. The numerical grids are designed to be finer near the fault and in the injection zone for more accurate capture of the CO₂ plume expansion and geomechanical responses.

Initial conditions for flow are assumed to be hydrostatic. The temperature is assumed to be 15°C, and the geothermal gradient is assumed to be 0.01225 °C/m. The water is assumed to be fresh at the surface and the mass fraction of salt increases with depth using a gradient of $3 \times 10^{-5} \text{ m}^{-1}$. The pressure at the top surface is assumed to be 101323 Pa and increases with depth assuming hydrostatic conditions, where the density of water varies with depth according to increasing temperature and salinity. Initial conditions for reactive transport are that the brine is in equilibrium with formation minerals. We assume that the sandstone reservoir layer is initially fully saturated with brine. This is a typical and reasonable assumption, although the formation could have initial gas saturations (e.g. natural gas). However, studying the effect of initial gas saturations is not the focus of this study.

The injection point is located in the reservoir near the southwest corner of the simulation domain and zero flux aqueous and gaseous boundary conditions are assumed for the south and west boundaries assuming symmetric flow and transport behaviors across these two boundaries. Aqueous boundary conditions are assumed to be hydrostatic at the north and east boundaries with a bottom aqueous pressure of 17.6 MPa, and zero flux for the gaseous phase is adopted at these boundaries assuming negligible flux of gases during the simulation period of 20 years after CO₂ injection starts. Zero flux boundary conditions are assumed above the nearly impermeable caprock and below the basement. An injection rate was set at 4.0 mmt/yr (metric million tons per year) in the injection reservoir interval along the injection borehole, with an injection period of 20 years. The assumed values of the initial formation permeability and porosity are given in Table 5. The permeability for the fault zones is assumed to be one percent of the permeability of the adjacent rocks, that is, the fault is hypothesized to act as a low-permeability barrier to flow and CO₂ migration. The porosity of the fault segments in the reservoir, caprock and basement, respectively are assumed to be the same values as the values assigned to the host layers. The initial values are 0.12 for the fault segment in the reservoir, and 0.051 for the fault segments in the caprock and basement. It is noted that analyses could also be conducted assuming higher permeability for the fault segments compared to the permeability for the surrounding rocks.

Figure 3. The reservoir unit was assumed to be 200-m thick and was overlain by a primary caprock. The location of reservoir is between -1240 m to -1040 m such that supercritical conditions predominate during the CO₂ injection period.

5.2 ABAQUS[®] 3D finite element model

Figure 4 shows the 3D ABAQUS[®] finite element model that exactly maps the STOMP-CO₂-R model. The ABAQUS[®] 3D mesh contains $27 \times 20 \times 37$ solid 8-node linear brick finite elements. The atmospheric pressure on the top surface and the lateral compression equal to the overburden due to gravity in the z-direction are schematically illustrated in Figure 4. Zero-normal displacements are applied on other boundary surfaces. In addition, gravity loading in the z-direction is applied inside the formation, and the fluid pressure computed by Equation (19) using STOMP-CO₂-R results are prescribed at the selected times during the STOMP-CO₂-R/ABAQUS[®] analysis. The ABAQUS[®] modeling domain is identical to the STOMP-CO₂-R domain that contains 3 layers including a shale basement, a sandstone reservoir and a shale caprock as well as a vertical fault. The vertical fault extending from the bottom to the top surface has three segments whose geomechanical properties vary with their locations inside the formation. Thus, the fault segment in the reservoir layer possesses different geomechanical properties from those for the basement and caprock. The fault was modeled using the same solid 3D finite elements as for the other formation layers. The elastic properties of the minerals that compose the formation rocks were based on (Mavko et al., 1998) and are provided in Table 4. Table 6 gives the initial homogenized elastic properties predicted by the EMTA model for the

different layers and fault segments of the formation illustrated in Figures 3 and 4. These initial elastic properties were calculated using the initial volume fractions given in Table 1 and the mineral elastic properties given in Table 4 except the value for the quartz elastic modulus in the fault. Typical fault structures are in general very complex and contain a single or multiple high-strain cores surrounded by a fractured damage zone (Faulkner et al., 2010). Accounting for the fractured damage zone that does affect the elastic modulus of the quartz matrix inside the fault, we assumed that the value of the elastic modulus of the quartz matrix in the fault was half of the value used for all the other areas of the formation. It is noted that other values for the damaged quartz matrix in the fault less than the elastic modulus for the undamaged quartz can be adopted, but for the purpose of our study to elucidate the geochemical-mechanical impact on formation rocks' geomechanical properties this assumption is acceptable. The friction angle considered for all the fault segments is 25° leading to a static friction coefficient of 0.47.

Figure 4. The 3D ABAQUS[®] finite element model that maps the STOMP-CO2-R model illustrated in Figure 3.

6. Results and discussion

6.1 Geochemical-mechanical effects

The STOMP-CO2-R/ABAQUS[®] simulator was used to analyze the model CO₂ reservoir illustrated in Figures 3 and 4. The selected times for the exchange data between STOMP-CO2-R

and ABAQUS[®] were sufficiently fine to accurately capture the variations of the governing variables for a given period of analysis (up to 20 years in this study). We performed a consistency check for the coupling solutions prescribing the exchange data between STOMP-CO2-R and ABAQUS to occur every 30 days, 100 days, 200 days, and every year to determine the convergence of the solution with the exchange data frequency refinement. The 30-day frequency for the exchange data has allowed to more accurately capture the fluid pressure evolution after the start of the injection. As the geochemical effect takes time to become significant, the 30-day frequency has then been maintained for the exchange data to achieve more accurate results. To understand the geochemical and combined geochemical-mechanical effects, comparative analyses of the same formation were also conducted using STOMP-CO2-R that provided only flow and geochemical solutions, or STOMP-CO2 sequentially coupled to ABAQUS[®] that accounted for the geomechanical effect but did not include geochemistry. All the analyses were performed on the Olympus supercomputer of PNNL's Institutional Computing Program. For the sequentially coupled STOMP-CO2-R/ABAQUS[®] simulations, one node with 32 CPUs and 64 GB memory was requested, and each 20-year-period simulation took about 3 days for completion.

Figures 5(a), 5(b) and 5(c) show the expansions of the CO₂ plume (gas saturation contours) in the reservoir layer at 20 years obtained from the analyses using STOMP-CO2-R, STOMP-CO2-R/ABAQUS[®] and STOMP-CO2/ABAQUS[®], respectively. For detailed visualizations of the plume expansions, the figures show the views through a cutting plane at $z = -1050$ m. The CO₂ plume from the STOMP-CO2/ABAQUS[®] solution is the largest (Figure 5(c)) and has already reached the North boundary at 20 years, and the one from the STOMP-CO2-R/ABAQUS[®] analysis is the smallest. All the plumes have crossed the fault at 20 years of injection. The relative size of CO₂ plumes resulting from the different analyses can be explained by examining the corresponding contours of intrinsic permeability given in Figures 6(a), 6(b) and 6(c). Figures 6(a) and 6(b) clearly show important reductions of permeability at 20 years predicted by STOMP-CO2-R and STOMP-CO2-R/ABAQUS[®], respectively. The CO₂ plume predicted by the geochemical analysis (Figure 5(a)) is larger than the one predicted by the geochemical-mechanical analysis although the difference between Figures 5(a) and 5(b) is little. This is because the geochemical effect on the permeability that controls the expansion of the CO₂ plume is dominant over the geomechanical effect. Similarly, little difference is observed for the contours of permeability presented in Figures 6(a) and 6(b): the reduction of permeability is mainly governed by geochemistry. The reduction of permeability predicted by the geochemical-mechanical analysis is more pronounced as the compressive stresses due to confining pressures have further reduced the permeability and thus slowed down the progression of the plume. The CO₂ plume predicted by the geomechanical analysis without geochemistry is the largest due to significantly higher permeability (Figure 6(c)) in this case compared to the other cases that included geochemistry.

Figure 5. Contours of CO₂ plume (gas saturation) in the reservoir at 20 years predicted by (a) STOMP-CO2-R only, (b) STOMP-CO2-R/ABAQUS[®] and (c) STOMP-CO2/ABAQUS[®].

Figure 6. Contours of intrinsic permeability at 20 years predicted by (a) STOMP-CO₂-R only, (b) STOMP-CO₂-R/ABAQUS[®] and (c) STOMP-CO₂/ABAQUS[®].

For comparison of results, Figure 6(c) uses the same scale for the contour of permeability as for Figures. 6(a) and 6(b), the small change in permeability predicted by the geomechanical STOMP-CO2/ABAQUS analysis is not quite noticeable. To evidence the geomechanical effect, Figure 7 illustrates the permeability evolution predicted by the geomechanical analysis for the injection location in the reservoir. Before the start of the injection and application of boundary conditions (time $t = 0$), the initial permeability prescribed for the reservoir layer is 10^{-13} m^2 , this is the *zero-stress* permeability. With the CO₂ injection and application of the boundary conditions and loadings involving gravity loading, fluid pressure and lateral compression, the permeability of the reservoir at the injection location is reduced to about $9.52 \times 10^{-14} \text{ m}^2$. As the fluid pressure at the injection location continues to increase during the first 2 months of injection (Figure 7), this has caused an increase in permeability at this location to a higher value. However, after a few months, the fluid pressure at the injection location predicted by the geomechanical analysis has progressively decreased, and this has levelled off the permeability just after a few months. It is noted that the fluid pressure at this location did not attain a level that could lead to permeability values higher than the initial zero-stress permeability.

Figure 7. Permeability evolution predicted by the geomechanical STOMP-CO2/ABAQUS[®] analysis for the injection location.

The distributions of porosity and mineral volume fractions predicted by STOMP-CO2-R/ABAQUS® at 20 years are given in Figures 8(a) to 8(f). Significant reduction of porosity due to chemical reactions led to a substantial reduction of intrinsic permeability illustrated in Figure 6(b). Figures 8(b) to 8(f) show that with respect to the initial values (Table 1) the volume fraction of albite has not varied noticeably while significant dissolution of anorthite and significant precipitations of calcite and kaolinite have occurred. The initial pH is 10, but drops immediately to a pH of 5 at the start of CO₂ injection. The pH drop results in faster anorthite dissolution. The pH then increases slowly with time due to the buffering effects of mineral precipitation and dissolution. The change in the quartz volume fraction was solely from the geomechanical origin due to the reduction in porosity. It has been mentioned in Section 3.1 that the pores were modeled as a separate inclusion phase embedded in the quartz matrix. Figure 9 gives the distribution of the homogenized elastic modulus of the reservoir layer at 20 years. Significant reductions of the reservoir elastic modulus are found over a large region in front of the fault and inside the fault segment. The precipitation of kaolinite, the least stiff mineral compared to the other hard phases (Table 4) was responsible for the reduction of the reservoir elastic modulus. However, the reduction in porosity combined with the precipitation of calcite, a much stiffer phase than kaolinite and also stiffer than anorthite, has balanced the effect of kaolinite precipitation on the reservoir elastic modulus. In the next section, the competing effects of reduced porosity and calcite/kaolinite precipitations will be discussed in combination with the CO₂ injection rate effect.

Albite Volume Fraction

Anorthite Volume Fraction

Calcite Volume Fraction

Figure 8. Contours of volume fractions at 20 years predicted by STOMP-CO2-R/ABAQUS® for (a) Porosity, (b) Albite, (c) Anorthite, (d) Calcite, (e) Kaolinite, and (f) Quartz.

Figure 9. Contour of predicted elastic modulus in the reservoir layer at 20 years.

The fluid pore pressure distributions in the formation obtained from STOMP-CO₂-R, STOMP-CO₂-R/ABAQUS[®] and STOMP-CO₂/ABAQUS[®] are presented in Figures 10(a), 10(b) and 10(c), respectively. First, all the contours show higher pressures in front of the fault. This is because the reservoir fault segment has much lower permeability than the reservoir rock. The initial values of permeability assigned to the reservoir and the reservoir fault segment are 10^{-13} m^2 and 10^{-15} m^2 , respectively. Thus, the fault has acted as a barrier to the expansion of the CO₂ plume. High fluid pressure buildup was predicted by the STOMP-CO₂-R analysis (Figure 10(a)), but the fluid pressure accumulation in front of the fault was the most important predicted by the geochemical-mechanical analysis (Figure 10(b)). In this case, substantial reduction of the intrinsic permeability has led to significant increase in fluid pressure at and beyond the injection location. The fluid pressure distribution predicted by the geomechanical analysis (Figure 10(a)) is lower than the geochemical or geochemical-mechanical predictions due to higher permeability in this case.

Figure 10. Distributions of pore fluid pressure at 20 years predicted by (a) STOMP-CO₂-R, (b) STOMP-CO₂-R/ABAQUS[®], and (c) STOMP-CO₂/ABAQUS[®].

To examine the geochemical or the combined geochemical-mechanical effects on the fluid pressure, **Figure 11** provides the fluid pressure evolutions at the injection location predicted by different analyses performed in this study. First, right after the start of the CO₂ injection, all the analyses predicted nearly the same level of fluid pressure attained. After the initiation period, **Figure 11** shows that the predicted fluid pressures dropped, and their evolutions diverged as time went on. The pressure drop was mainly caused by the increasing gas volumetric content. When gas saturation is close to 1, the increase in gas relative permeability is more than the decrease in aqueous relative permeability (Krevor et al., 2012); therefore, there is a net increase in the equivalent or effective fluid relative permeability, which results in a pressure drop. The drop in gaseous viscosity (which is dependent on pressure and temperature conditions) was also related to the reduction of resistance force and thus led to pressure decrease. After several years of injection, the significant reduction in the intrinsic permeability predicted by the geochemical and geochemical-mechanical solutions have brought the fluid pressure at the injection location up while the fluid pressure predicted by the geomechanical analysis continued to decrease as explained above. **Figure 11** also shows that the fluid pressure predicted by the geochemical-mechanical analysis is the highest. This was due to a larger reduction of the intrinsic permeability predicted by STOMP-CO₂-R/ABAQUS[®].

Figure 11. Evolutions of fluid pressure at the injection location predicted by STOMP-CO2-R/ABAQUS®, STOMP-CO2-R and STOMP-CO2/ABAQUS®.

Figure 12. Fluid pressures at 20 years along the x -direction at $y = 0$ and $z = -1230$ m predicted by STOMP-CO2-R/ABAQUS®, STOMP-CO2-R and STOMP-CO2/ABAQUS®.

Figure 12 reports the variations of the fluid pressure predicted from different analyses in the reservoir at 20 years along the x -direction (at $y = 0$ and $z = -1230$ m) from the injection location to the East boundary. Figure 11 clearly shows the buildup of fluid pressure in front of the fault as the fault with much lower permeability than the surrounding reservoir rocks has acted as a barrier to the fluid expansion in the x -direction. The buildup in fluid pressure predicted by the geochemical-mechanical analysis is the highest due to a substantial reduction of the intrinsic permeability in this case as discussed above.

Figure 13. Evolutions of pressure margin to fracture (PMF) predicted by STOMP-CO2-R/ABAQUS® and STOMP-CO2/ABAQUS® for the injection location.

The pressures margin to fracture (PMF) (Equation (22)) predicted by STOMP-CO2-R/ABAQUS® and STOMP-CO2/ABAQUS® for the injection location reported in Figure 13 exhibit different trends. At the start of the injection, both analyses predicted the same reduction of PMF due to the fluid pressure increase (illustrated in Figure 11). A reduction of PMF means that the least compressive effective principal stress (that defines PMF) is closer to zero. When PMF is equal to or exceeds zero, hydraulic fracture is predicted to occur (Jaeger and Cook, 1979). Figure 11 shows that after a few months, PMF predicted by the geochemical-mechanical analysis increased very slightly and then progressively decreased as a result of the fluid pressure buildup (Figure 11). On the other hand, PMF predicted by the geomechanical solution increased continuously after an initial reduction. Both solutions predicted PMF at the injection location significantly lower than zero for a period of 20 years, so hydraulic fracture was not predicted to

occur at this location. However, for longer periods of injection, PMF predicted by the
 geochemical-mechanical analysis is expected to further decrease. The reduction of the reservoir
 elastic modulus (Figure 9) is significant when examining this reduction in the context of the
 coupled hydro-geochemical-geomechanical process that is modeled in this paper. It causes a
 reduction of PMF that is further reduced by the increase in fluid pressure due to the reduction of
 permeability. Figure 13 shows a significant reduction of PMF predicted by the coupled hydro-
 geochemical-geomechanical analysis for the injection location where the reduction in elastic
 modulus is about 5% at 20 years of injection (at the injection rate of 4 mmt/yr). The PMF
 evolutions predicted by STOMP-CO2-R/ABAQUS[®] and STOMP-CO2/ABAQUS[®] for the
 locations in the fault segment of the reservoir layer and in the fault segment of the caprock near
 the reservoir are given in Figures 14 and 15, respectively. When the CO₂ plume has not yet
 reached the fault for about 10 years, the geomechanical and geochemical-mechanical solutions
 for PMF are identical, but as soon as the plume reached the fault, the norms of PMF (absolute
 value of PMF, $\text{abs}(\text{PMF})$) predicted by STOMP-CO2-R/ABAQUS have decreased as a result of
 higher fluid pressures due to reduced permeability. However, the reductions in PMF are very
 small, and the PMF solutions for these locations are quite similar.

Figure 14. Evolutions PMF predicted by STOMP-CO2-R/ABAQUS[®] and STOMP-
 CO2/ABAQUS[®] for a location in the fault segment of the reservoir layer.

Figure 15. Evolutions PMF predicted by STOMP-CO2-R/ABAQUS[®] and STOMP-CO2/ABAQUS[®] for a location in the fault segment of the caprock near the reservoir layer.

The contours of slip tendency factor on the vertical fault predicted by STOMP-CO2/ABAQUS[®] and STOMP-CO2-R/ABAQUS[®] at 20 years are shown in Figures 16(a) and 16(b), respectively. These figures show the contours in a vertical plan within the fault. The slip tendency factor predicted by both analyses using the static friction coefficient of 0.47 was very small (~ 0) due to its vertical position and the much stiffer reservoir layer than the basement and caprock leading to very low shear strains and shear stresses on the fault plan, and therefore the risk for the fault in the model formation to slip was negligible compared with 0.47. Due to lower effective normal stresses caused by higher fluid pressures, the values of slip tendency factor predicted by the geochemical-mechanical analysis are higher than those obtained from the geomechanical solution.

(a)

(b)

Figure 16. Fault slip tendency factor within the fault at 20 years predicted by (a) STOMP-CO2/ABAQUS[®] and STOMP-CO2-R/ABAQUS[®].

6.2 Injection rate effects

To further elucidate and understand the geochemical-mechanical effects on the formation behavior, it is important to examine the CO₂ injection rate effect on the fluid pressure, PMF, and mechanical properties of reservoir rocks and seals. To this end, the analyses of the same model formation (Figures 3 and 4) were performed by STOMP-CO2/ABAQUS[®] and STOMP-CO2-R/ABAQUS[®] considering an injection rate of 1 mmt/yr. Figure 17 reports the evolution of fluid pressure at the injection location obtained at this lower rate compared to the curve predicted at the higher rate (4 mmt/yr). The curves globally exhibit the same trend, however, reducing the injection rate has brought the fluid pressure down. The curve at higher injection rate shows a faster evolution of fluid pressure after 10 years of injection. Reducing the injection rate also has slowed down the expansion of the CO₂ plume (as compared to the contour illustrated in Figure 5(b) for the 4-mmt-rate case). In the low injection rate case, the plume shown in Figure 18 was still far away from the North boundary at 20 years.

The effect of the injection rate on the PMF is shown in Figures 19(a), 19(b) and 19(c) that compare the evolutions of PMF predicted at low and high injection rates at the injection location, in the fault segment of the reservoir layer, and in the fault segment of the caprock near the reservoir. Decreasing the injection rate has led to enlargements of PMF (in absolute values) in all the examined locations. The enlargement of PMF at the injection location was the most important. Long-term injection of CO₂ at high injection rates would increase the risk of fracture of the reservoir at the injection location. The enlargement of PMF in the fault segment of the reservoir layer was also significant, but a smaller enlargement of PMF was found in the fault segment of the caprock near the reservoir.

Figure 20 reports the evolutions of the reservoir elastic modulus as a function of the injection rate at the injection location (Figure 20(a)) and inside the reservoir fault (Figure 20(b)). At the injection location, the elastic modulus first decreased due to the precipitation of kaolinite, a softer mineral, however after many years of injection, the precipitation of calcite and significant reduction of porosity (Figure 21) have progressively stabilized the trend as clearly shown in Figure 20(a) that also compares the predicted modulus evolutions to an hypothetical linear one. The higher injection rate stabilized the reduction of the elastic modulus somewhat faster. Figure 20(b) shows that no change in elastic modulus is observed at 1 mmt/yr because the CO₂ plume has not yet crossed the fault. As soon as the CO₂ plume has reached the fault at 4 mmt/yr, precipitation of kaolinite reduced the reservoir fault elastic properties. However, it is expected that if the CO₂ injection continues at 4 mmt/yr after 20 years, precipitation of calcite and reduction of porosity would stabilize the modulus of the reservoir fault. The results reported in Figure 20 are the most important findings from this work. For the mineralogy and reaction system considered, the reservoir rock elastic modulus decreases at some extent (depending on the injection rate) due to the reactive transport of CO₂ but reaches a minimum after long periods of injection as a result of calcite precipitation and reduction of porosity.

Figure 17. Fluid pressure in the injection location as a function of the injection rate.

Figure 18. Contours of CO₂ plume (gas saturation) in the reservoir at 20 years of injection at 1 mm/yr predicted by STOMP-CO2-R/ABAQUS®.

720

(a)

(b)

721

(c)

Figure 19. Predicted PMF as a function of the injection rate (a) in the injection location, (b) in a location in the fault segment of the reservoir layer, and (c) in the fault segment of the caprock near the reservoir layer.

Figure 20. Predicted evolution of the elastic modulus as a function of the injection rate (a) in the injection location, and (b) inside the fault segment of the reservoir layer.

Figure 21. Evolution of porosity in the injection location at different injection rates.

7. Conclusions

This paper has modeled the reactive transport of CO₂ and its impact on the mechanical properties of the reservoir rocks and seals. Comparative analyses using different computational simulators including STOMP-CO₂-R, STOMP-CO₂-R/ABAQUS® and STOMP-CO₂/ABAQUS® were performed to study the hydro-geochemical, hydro-geochemical-mechanical, and hydro-geomechanical processes to differentiate their effects on the formation response. The results show that the fluid pressure distribution predicted by the hydro-geochemical-mechanical analysis was the most important due to substantial reduction of intrinsic permeability in this case. Increased fluid pressure has led to reduction of the fracture margin to fracture (in absolute values, $abs(PMF)$) at different examined locations, in particular, at the injection location. For the formation rocks considered, the analyses accounting for the hydro-geochemical-mechanical process have shown that long-term injection of CO₂ first reduced the elastic moduli of rocks due to a precipitation of kaolinite, a softer mineral. However, after many years of injection and depending on the injection rate, the evolutions of elastic moduli stabilize and seem to exhibit a trend to increase as a result of increased reduction of porosity combined with the precipitation of calcite. These findings mean that long-term injection of CO₂ will not cause continuous reduction of elastic moduli but the rock stiffness can stabilize after an initial period of reduction. For the faulted formation analyzed, the risk of the fracture of the caprock

seal is very unlikely as very small reduction of PMF was found due to the geochemical effect. Accounting for geochemistry in the hydro-geomechanical analysis led to a small increase in the fault slip tendency factor, but the effect also is very small and negligible. However, the CO₂ injection rate has a more important effect as increasing the injection rate has led to an increase in fluid pressure that significantly reduced the PMF in the reservoir layer and caprock.

At this stage of our work, the focus has been on the development of the computational tool that interfaces STOMP-CO2-R to ABAQUS[®] to solve the very complex problem of flow fully coupled to both geochemical and geomechanical processes and elucidate the effect of mineral composition change on the geomechanical properties of reservoir rocks and seals. We have then applied this tool in combination with the EMTA module implemented in ABAQUS[®] to a reservoir formation model containing a sandstone reservoir and a shale caprock and basement. As this is a model formation whose layers are composed of assumed initial volume fractions, the measured property data for the as-formed rock materials are not available. However, the EMTA was widely used for various structural or engineering materials and have been proved to be an efficient and accurate method to predict the homogenized elastic properties of a material from its constituent elastic properties and features. All the previous findings reported in the literature about EMTA have given us confidence in the application of this method to our present problem. In future work, mechanical testing can be performed to measure the elastic properties of typical reservoir rocks with known constituent properties and compositions and to compare the measured values to EMTA's predictions.

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Tables

Table 1. List of initial mineral volume fractions, potential secondary mineral phases, and their kinetic properties

Mineral	Composition	Sandstone Volume, %	Shale Volume, %	Surface Area, cm ² /g	r_{25} , mol/m ² s (a)	E_a kJ/mol (b)
Albite	NaAlSi ₃ O ₈	8.80	0.95	36.2	9.20E-13	69.8
Anorthite	CaAl ₂ (SiO ₄) ₂	8.80	0.95	36.2	7.59E-10	17.8
Calcite	CaCO ₃	0.88	0.95	36.9	1.55E-06	23.5
Kaolinite	Al ₂ Si ₂ O ₅ (OH) ₄	0.88	56.94	3860	6.61E-14	22.2
Quartz	SiO ₂	68.64	35.11	37.7	4.57E-14	90.1

(a) Palandri and Kharaka (2004)

(b) Xu et al. (2007)

Table 2. Mineral kinetic reactions and equilibrium constant temperature coefficients

Kinetic Reactions	log K_{eq} Temperature Coefficients				
	a	b	c	d	e
Albite = $AlO_2^- + Na^+ + 3SiO_2(aq.)$	4.39E+02	-2.87E+03	-3.56E-01	1.77E+05	-1.27E+07
Anorthite = $2AlO_2^- + Ca^{2+} + 2SiO_2(aq.)$	4.73E+02	-3.06E+03	-4.20E-01	1.82E+05	-1.21E+07
Calcite + $2H^+ = CO_2(aq.) + Ca^{2+} + H_2O$	3.78E+01	-2.33E+02	-3.59E-02	1.18E+04	-2.83E+05
Kaolinite = $2AlO_2^- + 2H^+ + H_2O + 2SiO_2(aq.)$	4.27E+02	-2.77E+03	-3.74E-01	1.58E+05	-1.11E+07
Quartz = $SiO_2(aq.)$	1.01E+02	-6.65E+02	-7.47E-02	4.36E+04	-3.28E+06

Table 3. Aqueous equilibrium reactions and equilibrium constant temperature coefficients

Equilibrium Reactions	log K_{eq} Temperature Coefficients				
	<i>a</i>	<i>b</i>	<i>c</i>	<i>d</i>	<i>e</i>
$AlO_2^- + 4H^+ = Al^{3+} + 2H_2O$	-3.61E+01	2.23E+02	3.32E-02	-4.49E+03	9.13E+05
$CO_2(aq.) + H_2O = H^+ + HCO_3^-$	1.05E+02	-6.71E+02	-1.09E-01	3.88E+04	-2.65E+06
$CO_2(aq.) + H_2O = CO_3^{2-} + 2H^+$	2.32E+02	-1.49E+03	-2.37E-01	8.41E+04	-5.56E+06
$CO_2(aq.) + Ca^{2+} + H_2O = CaCO_3(aq.) + 2H^+$	-3.97E+01	2.39E+02	3.34E-02	-1.09E+04	-6.14E+03
$Ca^{2+} + Cl^- = CaCl^+$	-1.31E+02	8.27E+02	1.33E-01	-4.66E+04	2.90E+06
$Ca^{2+} + H_2O = CaOH^+ + H^+$	5.64E-07	-1.29E+01	-3.09E-10	7.47E-05	-8.38E-03
$2H_2O + SiO_2(aq.) = 2H^+ + H_2SiO_4^{2-}$	1.01E-06	-2.30E+01	-5.52E-10	1.33E-04	-1.50E-02
$H_2O + SiO_2(aq.) = H^+ + HSiO_3^-$	5.73E+00	-1.37E+01	-3.54E-02	-8.17E+03	8.09E+05
$CO_2(aq.) + H_2O + Na^+ = 2H^+ + NaCO_3^-$	4.94E+01	-3.18E+02	-8.46E-02	2.00E+04	-1.94E+06
$CO_2(aq.) + H_2O + Na^+ = H^+ + NaHCO_3(aq.)$	1.11E+03	-7.07E+03	-1.03E+00	3.99E+05	-2.39E+07
$H_2O + Na^+ + SiO_2(aq.) = H^+ + NaHSiO_3(aq.)$	-1.29E+02	8.46E+02	9.42E-02	-5.57E+04	3.73E+06
$H_2O = H^+ + OH^-$	1.17E+02	-7.45E+02	-1.17E-01	3.92E+04	-2.64E+06

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Table 4. Mineral properties

Mineral	Density (g/cm ³)	Molecular Weight (g/mol)	Elastic Modulus (MPa)	Poisson Ratio
Albite	2.616	262.2230	69120	0.35
Anorthite	2.760	278.2073	69120	0.35
Calcite	2.710	100.0872	84293	0.317
Kaolinite	2.594	258.1604	3203	0.144
Quartz	2.648	60.0843	95756	0.064

Table 5. The major hydrological parameters’ values used in the STOMP-CO2 and STOMP-CO2-R models

Parameter	Value
Brooks and Corey, λ	0.8284
Aqueous residual saturation, $\bar{s}_m$	0.06143
Initial caprock porosity, ϕ	0.051
Initial caprock intrinsic permeability, k	1.0e-17 m ²
Caprock air entry pressure P_0	11.1 m
Initial reservoir porosity, ϕ	0.12
Initia; reservoir intrinsic permeability, k	1.0e-13 m ²
Reservoir air entry pressure, P_0	0.606 m

Table 6. The initial elastic properties predicted by EMTA for formation rocks.

	Elastic Modulus (MPa)	Poisson's Ratio
Basement	26080	0.1405
Basement Fault	15000	0.1388
Reservoir	78380	0.3484
Reservoir Fault	46660	0.1571
Caprock	26080	0.1405
Caprock Fault	15000	0.1388

Table 7. Parameters used in the failure criteria

Rock Tensile Strength (MPa)	0
Cohesion Coefficient, c_0	0
Friction Angle, φ	25