Thermal Impact of CO₂ Injection on Geomechanical Response at the FutureGen 2.0 Site: A Three-dimensional Thermo-geomechanical Approach

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Abstract: The impact of temperature variations of the injected CO₂ on the mechanical integrity of a reservoir is an important problem but rarely addressed in the design of a CO₂ storage site. In this study, a three-dimensional (3D) thermo-geomechanical approach was developed to evaluate the possibility of fracturing the FutureGen 2.0 site due to injection of CO₂ at different temperatures. The approach sequentially coupled the STOMP-CO2 code for flow and thermal analyses to the ABAQUS[®] finite element package for performing thermo-geomechanical analyses of this site. The 3D STOMP-CO2 model of the FutureGen 2.0 site contains four horizontal wells and variable layer thickness, flow and thermal properties. The 3D ABAQUS[®] finite element (FE) model for thermo-geomechanical analysis which exactly maps the STOMP-CO2 model contains variable thermo-geomechanical properties. **Boundary conditions were prescribed to the FE model to achieve the strike-slip faulting stress regime observed at the FutureGen 2.0 site.** The STOMP-CO2 model takes into account the results from modeling the heat exchange between the environment and CO₂ during its transport in the pipeline and injection wells before reaching the reservoir, as well as its interaction with the reservoir host rock. Injection temperature in the reservoir, whose initial temperature was 36°C, was varied, and two cases were simulated and modeled: 28°C, the minimum possible temperature considered as an extreme case since it corresponds to winter conditions maintained during the 20 years of the injection, and 47°C that represents the annual average injection temperature. **The STOMP-CO2/ABAQUS[®] analyses indicate lower injection temperatures approaching 28°C could locally induce shear slip activation close to the wells and confined to the reservoir. Thermally induced hydraulic fracture is not expected for the 28°C - 47°C injection temperature range or higher.**

Keywords: CO₂ reservoir; geomechanics; geomechanical modeling; hydraulic fracture; shear slip activation; elastic modulus; thermal stress

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1. Introduction

Geological sequestration of CO₂ in deep saline aquifers is promising for long-term CO₂ storage. The success of such storage is associated with the absence of leakage through natural pathways, wellbores, and fracture/fault systems. Properly sited and managed geologic carbon storage in deep saline formations remains a safe option to mitigate anthropogenic climate change (Vilarrasa and Carrera, 2015). Among the many factors that affect the leakage rates are formation flow and transport attributes, the pressure buildup and the geomechanical stresses due to injection. One important factor, the injection temperature, can also be important in practice. If CO₂ is injected at a temperature different from the temperature in the aquifer, additional stresses develop due to thermal expansion and contraction (Gor and Prévost, 2013). (Vilarrasa et al., 2013) found that the thermal effect can be pronounced for large temperature contrasts and stiff rocks, and the temperature decrease close to the injection well induces a stress reduction due to thermal contraction of the media. This can lead to shear slip of pre-existing fractures in the aquifer for large temperature contrasts in stiff rocks. The effect of shear slip can be advantageous when it occurs within the aquifer, because it enhances permeability and thus CO₂ injectivity. Rutqvist (2015) discussed observations of temperature and chemically mediated fracture closure and its effect on fractured rock permeability, and showed significant temperature-driven fracture closure even under constant stress.

However, the impact of temperature variations of the injected CO₂ on the mechanical integrity of a reservoir is a problem rarely addressed in the design of a CO₂ storage site, although some previous studies of CO₂ storage discussed the thermal stress issues related to CO₂ injection (Bissell et al., 2011; Comerlati et al., 2006; Freeman et al., 2008; Goodarzi et al., 2010; Hou et al., 2012; Kim and Hosseini, 2009; Lucier et al., 2006; Rutqvist et al., 2007; Rutqvist et al., 2002; Winterfeld and Wu, 2012). It is still a common practice in geologic carbon storage applications to neglect thermal effects (Bao et al., 2013; Kano et al., 2013; Rutqvist et al., 2013; Yamamoto et al., 2013). The findings of previous studies are still open, for example, Preisig and Prévost (2011) studied the effects of injecting CO₂ at a lower temperature than the formation at In Salah, and observed the possibility of tensile fracturing in the lowest part of the caprock within the first 3 years of injection; while Gor and Prévost (2013) studied the same site but stated that the lowest part of the caprock could be fractured after 12 years of injecting CO₂ at a temperature ~40°C – 50°C lower than the reservoir temperature. Such differences in their simulation results of the In Salah modeling are due to the initial stress states that they consider. Vilarrasa et al. (2015) used input parameters very similar to those used by Gor et al. (2013); however, Vilarrasa et al. (2015) predict shear failure of the lowest part of the caprock, and do not predict tensile fracturing as predicted by Gor et al. (2013). More complete understanding and systematic evaluation of thermal effects due to CO₂ injection are needed to guide CO₂ injection and storage design.

In the FutureGen 2.0 project, the CO₂ captured at the oxycombustion power plant was planned to be transported through a 48 km long underground pipeline to four horizontal injection

wells located on a single well pad in Morgan County, Illinois (Figure 1). The wells were to be drilled into a zone of high permeability within the upper portion of the Mount Simon Sandstone, a formation that underlies the whole central Illinois. As much as 1.1 metric million tons (MMT) of CO₂ was to be injected annually over 20 years. As thermal impact of the CO₂ injection temperature is an important problem, documentation of the analyses performed to support the FutureGen project will also help other carbon storage projects that are currently in the planning stage.

Figure 1. Conceptual design of the proposed FutureGen 2.0 CCS project, Illinois, USA.

The hydro-thermo-poroelastic approach used in our paper describes the coupled process between thermo-mechanics and flow in porous media. It belongs to the Biot's generalized theory for 3D porous media (Biot, 1941). Although there is significant research in this area, the numerical solution for the Biot partial differential equations is still challenging. In the fully coupled approach, the coupled nonlinear system of equations are discretized and solved simultaneously, typically using a Newton-Raphson's scheme. According to many authors (Settari and Mourits, 1998; Thomas et al., 2003; Jha and Juanes, 2007; Jha and Juanes, 2014), the simulation of flow and geomechanics for realistic fields become computationally very expensive. The fully coupled approach leads to algebraic systems which can be quite difficult to solve with very large number of unknowns in real 3D applications (Ferronato et al., 2010). On the other hand, there are sequential approaches, which couple flow to geomechanics sequentially or iteratively, can also offer as accurate solutions as the fully coupled approach if tight convergence criteria are prescribed. The fully coupled and sequentially coupled flow-geomechanics approaches were discussed by Prevost (2013) and Kim et al. (2011). As the sequentially coupled approach solves separately in a sequential way the fluid flow equations and the mechanical

problem (e.g., Rutqvist and Tsang, 2002; Rutqvist et al., 2007), it offers the flexibility to use separate simulators for each sub problem.

The accurate assessment of the risks associated with potential leakage of injected CO₂ and the design of effective CO₂ reservoir systems require numerical analyses of the multifluid flow process coupled with the thermo-geomechanical behavior of underground rocks. For practical reasons, under the National Risk Assessment Partnership (NRAP) program, PNNL has developed a sequentially coupled multifluid-flow/geomechanical approach to analyze prototype CO₂ reservoirs to determine stress and strain distributions as well as the risks associated with fault reactivation caused by rock deformation under increasing injection pressure. The developed capability uses PNNL's STOMP-CO₂ multifluid flow simulator (White et al., 2012; White and Oostrom, 2006) that is interfaced with the commercial ABAQUS[®] finite element packages. In this paper, STOMP-CO₂ handles flow and thermal solutions while ABAQUS[®] performs geomechanical modeling accounting for thermal stresses. The STOMP-CO₂/ABAQUS[®] simulator is efficient to perform 3D analyses of complex-geometry formations (like the FutureGen 2.0 site) while achieving meaningful numerical solutions.

In this paper, the temperature at the bottom of the injection well was first determined. A PNNL computer code named CO₂Flow was specifically developed for this purpose. CO₂Flow can rigorously solve energy and momentum balances for CO₂ in pipelines and injection wells while considering changes in fluid state over the relevant conditions. Based on CO₂Flow's results for the injection temperature that could vary between 28°C and 47°C (as previously reported in Bonneville et al., 2014) compared to the initial average temperature in the well region of the reservoir of about 36°C as measured in-situ (Alliance, 2012), an evaluation of the potential thermal impact of CO₂ injection was performed in this work using the STOMP/ABAQUS[®] coupled simulator for two cases: 28°C and 47°C. **The measured in-situ stresses at selected depths from Cornet (2014) were explored to determine the geomechanical boundary conditions to achieve the strike-slip faulting stress regime.** The purpose of the analysis was to identify the potential for fracturing of the reservoir and/or caprock due to thermal stresses induced by injection of CO₂ at these temperatures. The strength of this paper is that the analysis of thermal effects has been conducted for a real (planned) CO₂ injection site to be considered in the design of the actual injection. A number of previous studies on thermal effects, with the exception of studies associated with the In Salah storage site, were generic. In this paper, site specific properties and conditions have been used, including in-situ measured stresses, consideration of the surface pipe-lines, real well geometry and site specific geological layers and properties.

2. Pipeline and Injection Tubing Model: CO₂Flow

Design and planning of a CO₂ storage facility requires an understanding of the changes in fluid temperature and pressure along the entire flow path, including the injection well tubing and any pipeline that is needed to transport the fluid from its source to the storage site. The fluid state (temperature and pressure) varies along the length of pipe and tubing due to hydrostatic effects,

frictional losses, and thermal effects (Lu and Connell, 2008). The same equations govern transport phenomena in the pipeline carrying the fluid to the wellhead as in the well injection tubing, although different terms may dominate, depending upon parameters such as pipe diameter, pipe orientation, and the nature of heat transfer to the surroundings.

The CO2Flow computer program was written to model the changes in compressed CO₂ temperature and pressure as it moves through pipelines and well tubing. This is accomplished by explicit momentum and energy balances over a discrete number of pipe segments. A complete description of the model can be found in Stewart et al. (2012), and this model was also used and discussed in Bonneville et al. (2014). The computer model uses the well-established Span and Wagner (1996) state equations for CO₂ to describe changes in fluid properties. The program can calculate flow behavior of CO₂ as liquid, gas, or supercritical fluid; but cannot currently handle phase transitions or multi-phase flow. Proper functioning of the CO2Flow program has been checked using hand calculations corresponding to simple test cases, and predictions for full well simulations have been validated by comparison to data from injection tests at the American Electric Power (AEP) Mountaineer test site near New Haven, West Virginia.

Heat exchange between the moving fluid and its surroundings may also be accounted for in the model. In the case of a buried pipeline, the rate of heat transfer depends primarily upon the temperature of the surroundings and the soil thermal conductivity; but also upon the fluid velocity, which is in turn a function of the pressure along the flow path between the plant and wellhead. In the case of the injection well, significant heat transfer can also occur between the injected fluid and the surrounding rock when injection is first initiated. However, the rate of heat transfer is expected to decrease over time, as a zone of rock around the well moves closer to thermal equilibrium with the fluid. A limiting case after long time periods of steady injection is therefore considered to be adiabatic flow of fluid in the well. Under these conditions, the fluid temperature moving down the well can still change due to Joule-Thomson effects (Thu, 2013).

The FutureGen 2.0 project design included a 45.4 km pipeline from the power plant to the injection site. Here the flow would be divided among four injection wells. The design of each well included a straight vertical segment to a depth of 970 m, followed by a curved segment having a radius of 253 m, and finally a horizontal well segment. The design called for the perforated well section to begin in the curved segment, which would place the top of the injection interval somewhat higher than the horizontal portion of the well. The perforations were to begin at a linear distance of 248 m along the curved segment, corresponding to a total depth of 1181 m below the ground surface. The model also included a 56 m increase in elevation along the pipeline from the plant to the injection site.

The temperature of the CO₂ entering the pipeline was specified as a design parameter of the separation plant. STOMP-CO₂ was used to calculate the pressure at the end of the injection tubing (at the top of the injection interval) required to push the CO₂ into the repository at the required rate. This pressure would vary over the course of injection operations as the formation is pressurized, and then as the pressure in the formation relaxes during outages. Maximum

required pressures at the top of the injection interval were used for most design purposes. The well system was designed assuming that the maximum required pressure was near the specified pressure limit, which was 90% of the formation fracture pressure. Since the temperature was specified at one end of the flow path through the pipeline and injection tubing and pressure at the other, the calculation started with an assumed pressure at the plant, and then iterated this pressure until the pressure of the fluid at the top of the formation was equal to the required value.

Well and pipeline flow simulations were carried out for a number of conditions, covering expected injection pressures, fluid flow rates, and seasonal temperature variations. Soil thermal conductivity depends upon the soil composition and the water content, which will vary with the season. Since soil thermal conductivities at the site had not been characterized, a range of values were used in the simulations to bracket the rate of heat transfer expected in the pipeline. Assuming high moisture content in winter (and therefore higher thermal conductivities) and low moisture content in the summer (and therefore lower thermal conductivities) leads to a maximum variation in heat transfer over the course of the year. Extreme high and low values of 2.6 and $0.35 \text{ W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$ are suggested by Frank Kreith et al. (2011). High and low values of 1.25 and $0.50 \text{ W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$ are likely more realistic for the agricultural soil and moisture ranges expected along the FutureGen 2.0 pipeline route. The conditions chosen to be most representative of long, relatively steady injections were those of nominal flow rate (1.1 Mt/yr) and maximum pressure at the top of the injection interval (90% of estimated fracture pressure).

Table 1 shows input parameters for a representative set of cases examined using the CO2Flow program. Table 2 shows calculated (or specified) CO₂ temperatures and pressures at the plant, wellhead, and top of the injection interval for summer and winter seasons. The total CO₂ flow is assumed to be split evenly between four identical wells. Adiabatic conditions are assumed around the non-perforated sections of the wells, corresponding to conditions expected after long, steady-state operation. This calculation does not include any pressure drop due to throttling or control valves, which would likely be included in the final system in order to control the pressure and distribute flow between the four injection wells. Any pressure drop across valves at the wellhead would result in a corresponding increase of pressure in the pipeline and at the power plant.

The extreme values of soil conductivity led to a range of temperatures at the top of the injection interval of 28 to 55.4°C , corresponding to a yearly average value of 42°C . A more realistic range of soil conductivities for the planned pipeline route resulted in an average fluid temperature of 47°C at the top of the injection interval. This is a reasonable estimate of the actual injection temperature, considering that the thermal mass of the rock around the well will tend to buffer any transient extremes. The lowest injection temperature at the reservoir, 28°C , and the average temperature, 47°C , are used in the geomechanical modeling analysis described below.

The CO₂ temperature at the top of the injection interval is expected to be colder than the formation in the winter, but in the summer average CO₂ temperatures are expected to be somewhat higher. As shown in Lu and Connell (2008), temperature profiles along the length of the well are expected to be quite nonlinear during a CO₂ injection. Where the downhole fluid temperature ends up with respect to that of the formation will depend not only upon the fluid

temperature at the wellhead, but upon geothermal gradient, well depth, pressure along the well (which depends on the tubing diameter), and duration of the injection operation. The relatively high temperatures predicted for the fluid exiting the injection tubing in the summer, compared to the formation temperature at depth, are due in part to the high planned effluent temperatures from the FutureGen 2.0 CO₂ capture plant, along with the relatively low geothermal gradient existing at the FutureGen 2.0 site.

Table 1. Input Parameters for Example Pipeline and Well Case (Bonneville et al., 2014).

Parameter	Value	Unit
Average annual flow rate	1.10	Mt/yr
System availability fraction	0.85	
Maximum required injection pressure (at top of perforated well section)	15.63	MPa
Pipeline length	45.4	km
Pipeline slope (rise/run)	0.00124	
Pipeline element length (for numerical integration)	40	m
Fluid temperature at plant	45	°C
Average soil surface temperature (summer)	26.2	°C
Average soil surface temperature (winter)	1.4	°C
Soil thermal conductivity (summer)	0.35–0.5	W.m ⁻¹ .K ⁻¹
Soil thermal conductivity (winter)	1.25–2.6	W.m ⁻¹ .K ⁻¹
Pipeline cover depth	1.52	m
Pipeline inside diameter	0.257	m
Pipeline outside diameter	0.273	m
Length of vertical well segment	970.5	m
Well curved segment radius of curvature	253	m
Distance along curved segment to perforations	248	m
Well element length (for numerical integration)	1	m
Injection tubing inside diameter	0.074	m
Pipe absolute roughness (pipeline and well tubing)	4.6×10^{-5}	m

Table 2. Calculated Fluid Conditions at Various Points Assuming Soil Conductivities of $2.6 \text{ W.m}^{-1}.\text{K}^{-1}$ in Winter and $0.35 \text{ W.m}^{-1}.\text{K}^{-1}$ in Summer (Bonneville et al., 2014).

Location	Temperature ($^{\circ}\text{C}$)		Pressure (MPa)	
	Winter	Summer	Winter	Summer
Plant	44.7	44.7	8.55	11.14
Wellhead	17.6	39.2	6.79	9.55
Top of injection interval	28.0	55.4	15.63	15.63

3. Multiphase flow and thermal model

The STOMP-CO₂ code solves conservation equations for component mass (i.e., water, CO₂, and salt) and energy on a structured orthogonal grid (White et al., 2012; White and Oostrom, 2006) with the options to simulate transient multiphase flow and transport associated with CO₂ injection. The conservation equations are expressed as partial differential equations. Each conservation equation is solved for a primary variable. The STOMP-CO₂ simulator assumes non-isothermal conditions and solves four coupled conservation equations: water mass, CO₂ mass, salt mass, and thermal energy. The collection of constitutive equations that describe the phase conditions, phase compositions, and phase densities, assuming phase equilibria, are referred to as the equations of state. For the range of temperature and pressure conditions anticipated for geologic sequestration projects, five phases are possible: 1) water-rich liquid (aqueous), 2) CO₂-rich phase, 3) CO₂ aqueous phase, 4) clathrated CO₂ (hydrate), and 5) crystalline salt (precipitated salt). The equations of state express: 1) the existence of phases given the temperature, pressure, and water, CO₂, and salt concentration, 2) the partitioning of components among existing phases, and 3) the density of the existing phases. The primary variables and the equation-of-state secondary variables are the foundation for computing the remaining thermodynamic and transport secondary variables.

The STOMP-CO₂ simulation is non-isothermal and involves energy transfer. The energy conservation equation equates the time rate of change of energy within a control volume with the flux of energy crossing the control volume surface. In the STOMP-CO₂ code, thermal energy is partitioned, according to thermal equilibrium conditions, among the fluid and solid phases. The thermal capacitance of unconnected pore space, represented by the difference between the total and diffusive porosity, is computed assuming it is filled with liquid water. Heat transfer occurs by advection of phase mass, diffusion of component mass and thermal diffusion through the fluid and solid phases. Heat transfer by hydraulic dispersion of flowing fluid phases is neglected. Enhanced vapor transport is incorporated through enhancement factors for component diffusion through the gas phase. Energy associated with component mass sources is included as internal

heat generation sources. Reference states for enthalpy and internal energy are component dependent. Latent heat transport is considered through vapor transport through the gas phase and equilibrium thermodynamics.

Phase equilibria calculations in STOMP-CO2 use the formulations of Spycher et al. (2003) for temperatures below 100°C and Spycher and Pruess (2010) for temperatures above 100°C, with corrections for dissolved salt. If the concentration of dissolved CO₂ in the aqueous phase exceeds the solubility limit, then the phase condition switches to aqueous and mobile gas. In the aqueous and mobile gas phase condition, two phases exist; the aqueous phase and the CO₂ predominate phase (gas), which can be supercritical or subcritical CO₂, or subcritical liquid.

In multi-phase systems, thermal conduction through the gas phase is neglected, because of the relatively low thermal conductivity of gas compared with the solid and liquid phases. For geologic media, the thermal conductivity of the solid phase is frequently anisotropic; therefore the effective thermal conductivity of a multiple-phase geologic-media system is computed as anisotropic. The thermal conductivity of liquid water is computed as a function of temperature and pressure from the steam table formulation. Thermal conductivity for aqueous solutions of sodium chloride is computed as a function of temperature, pressure, and salt concentration.

4. Thermo-geomechanical model

The poroelastic constitutive relations for rocks implemented in the STOMP-CO2/ABAQUS® tool were enhanced with consideration of thermal stresses due to temperature variations and thermal expansion behavior of the formation layers. The geomechanical behavior of rocks was assumed to be isotropic. The following discussion is written in standard geomechanical terms that apply to both isotropic and anisotropic stresses and materials. The mechanical calculations were all performed assuming isotropic behavior because anisotropic data were not available for the material properties. The thermo-poroelastic constitutive equations in the principal stress axes system are given by Coussy (2007), Coussy (2011) and Aichi and Tokunaga (2012):

$$\sigma_{ij} = C_{ijkl}(\varepsilon_{kl} - \varepsilon_{kl}^{\text{th}}) - \alpha_{ij}P = C_{ijkl}\varepsilon_{kl} - \alpha_{ij}P - C_{ijkl}\beta_{kl}\Delta T \quad (1)$$

where C_{ijkl} is the stiffness tensor of the solid rock material without fluid, i, j, k , and l are the indices denoting the tensor components, and σ_{ij} and ε_{ij} are mechanical stress and total strain tensors, respectively. Tensile stresses are positive. $\varepsilon_{ij}^{\text{th}} = \beta_{ij}\Delta T$ is the thermal strain tensor with β_{ij} the thermal expansion coefficient tensor and ΔT is the temperature change. α_{ij} denotes the Biot's tensor (Biot and Willis, 1957). The assumption for isotropic rocks leads to $\alpha_{11} = \alpha_{22} = \alpha_{33}$ and $\alpha_{ij} = 0$ with $i \neq j$. Also, $\beta_{11} = \beta_{22} = \beta_{33} = \beta$; the values of the thermal expansion coefficient for the different layers of the formation are given in Table A1 of the Appendix. In this

work, the Biot parameter was unknown, so a value of $\alpha_{11} = \alpha_{22} = \alpha_{33} = 1$ was used for all layers. 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):

$$P = S_a P_a + (1 - S_a) P_g \quad (2)$$

Both the aqueous and gas pressures contribute to the fluid pressure, P . In addition, we used a power-law permeability model (e.g., Chin et al., 2000, Cappa and Rutqvist, 2011) that relates the intrinsic permeability to the porosity:

$$k = k_1 (\phi / \phi_1)^n \quad (3)$$

where n denotes the power-law exponent; k_1 and k are the initial and current permeability values; and ϕ_1 and ϕ are the initial and current porosities, respectively. A value of $n = 5.6$ was used based on Chin et al. (2000) and was applied to all layers in this work. The porosity is computed in terms of the volumetric strain, ε_v as (Chin et al., 2000, Cappa and Rutqvist, 2011)

$$\phi = 1 - (1 - \phi_1) e^{-\varepsilon_v} \quad (4)$$

with $\varepsilon_v = \varepsilon_{ii} = \varepsilon_{11} + \varepsilon_{22} + \varepsilon_{33}$.

The capillary entry pressure is computed in terms of the air-entry pressure, P_0 , permeability and porosity based on a relation by (Leverett, 1941) also used by (Rutqvist and Tsang, 2002):

$$P_c = P_0 \sqrt{k_1 / \phi_1} / \sqrt{k / \phi} \quad (5)$$

From Eq. (1), the principal effective stresses are computed as:

$$\sigma'_{ij} = \sigma_{ij} + \alpha_{ij} P = C_{ijkl} (\varepsilon_{kl} - \beta_{kl} \Delta T) \quad (6)$$

The principal effective stresses also determine the Mohr-Coulomb (Jaeger-Cook, 1979) fracture criterion according to which hydraulic fracture could develop as soon as the fluid pressure exceeds the least compressive principal stress, assuming zero-tensile strength. 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):

$$PMF = \text{Max}(\sigma'_{11}, \sigma'_{22}, \sigma'_{33}) \quad (7)$$

If the formation contains faults, the slip tendency factor on the fault plane is calculated using the Coulomb criterion (Jaeger and Cook, 1979): $\tau = c_0 + \mu_s \sigma'_n$ 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* S_f on the fault plan is equal to or exceeds μ_s :

$$S_f = \frac{\tau}{\sigma'_n} \geq \mu_s \quad (8)$$

μ_s is defined in terms of the friction angle φ as $\mu_s = \tan(\varphi)$.

Pre-existing faults or discontinuities were not detected at the FutureGen 2.0 site. In this paper we have used a shear-slip reactivation criterion derived by Rutqvist (2012) assuming a friction angle of $\varphi = 30^\circ$:

$$\sigma'_H \geq \sigma'_{Hc} = 3\sigma'_h \quad (9)$$

where σ'_H and σ'_{Hc} are the maximum and critical maximum compressive horizontal effective stresses, respectively. σ'_h is the minimum compressive horizontal stress. Relation (9) can be expressed in terms of a strength-to-stress margin as (Rutqvist, 2012):

$$SSM = \sigma'_{Hc} - \sigma'_H = 3\sigma'_h - \sigma'_H \quad (10)$$

according to which shear slip occurs if SSM is equal to or less than zero.

5. STOMP-CO2/ABAQUS computational procedure

The thermo-geomechanical analysis of the FutureGen 2.0 site discussed in the following sections was performed using the STOMP-CO2/ABAQUS[®] simulator. The thermo-poroelastic constitutive relations described in the previous section and the interface for the exchange data between these codes were implemented in ABAQUS[®] using user subroutines. The STOMP-CO2/ABAQUS[®] coupled analysis is executed sequentially in series. This means that for a given period of analysis the exchange data between STOMP-CO2 and ABAQUS[®] occurs at selected times prescribed in advance, with a STOMP-CO2 execution 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/ABAQUS[®] simulator. For the analysis of a geological formation, a STOMP-CO2 model of the formation is built to perform the thermo-hydrological simulation of the CO₂ flow in the formation that is a complex multilayer system containing a CO₂ reservoir between basement and caprock layers. An ABAQUS[®] finite element model of the same formation is built that exactly maps the STOMP-CO2 grid allowing the exchange of data between STOMP-CO2 and

ABAQUS[®]. At selected times, STOMP-CO2 provides ABAQUS[®] with the coordinates, aqueous pressure and saturation, gas pressure and saturation, porosity as well as the intrinsic permeability at each STOMP-CO2 cell center. Those cell centers are also ABAQUS[®] finite element centroids. Using STOMP-CO2 results as input, ABAQUS[®] integrates the thermo-poroelastic constitutive relations according to Eqs. (1), (2) and (6). After updating the stresses, the pressure margin to fracture is computed by Eq. (7). At each selected time, ABAQUS[®] provides STOMP-CO2 with the updated permeability, porosity, and capillary entry pressure based on Eqs. (3), (4) and (5), respectively.

Figure 2. STOMP-CO2/ABAQUS computational procedure.

6. STOMP-CO2 model

6.1 Model setup

The STOMP-CO2 (H2O-CO2-NaCl-Energy) model for the FutureGen 2.0 site was fully three-dimensional (3-D), with four horizontal wells diverging from a single vertical well and variable layer thicknesses. The modeling domain spans an area of 166 km x 166 km, with depth ranging from 290 m to 2110 m. The domain is discretized into 60 x 60 x 31 numerical grid cells (Figure 3a), following the stratigraphic structure from the available field survey information. The grids are refined near the center of the domain, where the four injection wells are located. There are four horizontal wells that radiate from the central injection point (Figure 3b). Each horizontal well has an internal well-bore radius of 0.1143 m; an injection mass rate of 6.5132×10^{-4} Mt/day (7.54 kg/s) for two of the wells and 1.0855×10^{-3} Mt/day (12.56 kg/s) for the other two wells designed with larger extensions; and maximum well-top pressure of 15.53 MPa. STOMP-CO2 coupled well module specifically computes the flow rate from a given well to adjacent cells

based on the pressure gradient and cells equivalent permeability. The well location and radius information are used to identify the surrounding cells. Injection temperature was varied, with two cases simulated and modeled: 28°C and 47°C. We adopted the Brooks and Corey model with gas entrapment Webb extension for the saturation function (Brooks and Corey, 1966; Webb, 2000) and Burdine porosity distribution model for aqueous/gas relative permeability function (Burdine, 1953).

(a)

Figure 3. (a) The STOMP-CO₂ grid of the FutureGen 2.0 site study domain, (b) The four horizontal injection wells.

Table 3 provides the names, positions and thicknesses of all the layers considered for the model. Figures 4 and 5 respectively present the initial values of the permeability and porosity for all the layers through the formation depth along a vertical direction containing the vertical portion of injection wells. Table A1 in the Appendix provides the relevant initial property values for all the layers. It is noted that uniform flow and geomechanical properties were assigned to each varying-depth layer. STOMP-CO₂ analysis used the anisotropic intrinsic permeability with components $k_{xx} = k_{yy}$ and k_{zz} . The norm value k of the permeability tensor was used in the geomechanical analysis by ABAQUS[®] where it is updated based on Equation (3). $k_{xx} = k_{yy}$ and k_{zz} were then updated proportionally in the coupled STOMP-CO₂/ABAQUS[®] analysis from the updated value of k .

Table 3. Names, thicknesses and positions of the layers in the formation. CO₂ is injected within the MtSimon11 and MtSimon17 layers.

Top Depth (m bgs)	Bottom Depth (m bgs)	Thickness (m)	Aggregate Layer
936.3	988.7	52.4	Franconia
988.7	1010.6	21.9	Davis-Ironton
1010.6	1043.9	33.2	Ironton-Galesville
1043.9	1069.8	25.9	Proviso4_5
1069.8	1091.7	21.9	Proviso1_3
1091.7	1125.3	33.5	Lombard12_14
1125.3	1144.9	19.7	Lombard8_11
1144.9	1152.1	7.2	Lombard5_7
1152.1	1169.8	17.7	Lombard1_4
1169.8	1172.8	3	Elmhurst7
1172.8	1175.8	3	Elmhurst6
1175.8	1178.9	3	Elmhurst5
1178.9	1183.2	4.3	Elmhurst4
1183.2	1184.4	1.2	Elmhurst3
1184.4	1187.4	3	Elmhurst2
1187.4	1191.1	3.7	Elmhurst1
1191.1	1199.0	7.9	MtSimon17
1199.0	1201.1	2.1	MtSimon16
1201.1	1205.1	4	MtSimon15
1205.1	1211.2	6.1	MtSimon14
1211.2	1219.7	8.5	MtSimon13
1219.7	1226.1	6.4	MtSimon12
1226.1	1233.1	7	MtSimon11
1233.1	1239.9	6.7	MtSimon10
1239.9	1246.6	6.7	MtSimon9
1246.6	1253.9	7.3	MtSimon8
1253.9	1260.9	7	MtSimon7
1260.9	1270.3	9.4	MtSimon6
1270.3	1294.1	23.8	MtSimon4_5
1294.1	1321.5	27.4	MtSimon2_3
1321.5	1346.5	25	MtSimon1

Figure 4. Initial values of permeabilities assigned for the layers in the model: A uniform value was assigned to each varying-depth layer. CO₂ is injected between depths 1191 m and 1233 m.

Figure 5. Initial values of the porosity as functions of depth assigned for the layers in the model: A uniform value was assigned to each varying-depth layer. CO₂ is injected between depths 1191 m and 1233 m.

Figure 6. Initial hydrostatic pressure distribution.

Figure 7. Initial temperature distribution.

6.2 Initial and boundary conditions

The initial conditions are required for STOMP-CO2 flow and geothermal analysis. The geothermal gradient was assumed to be $1.22 \times 10^{-2} \text{ }^{\circ}\text{C/m}$, which was estimated based on site-specific static borehole flow meter/fluid temperature survey in 2012. The reference salt mass fraction was assumed to be 4.75%. The initial pressure and temperature distributions are illustrated in Figures 6 and 7, respectively. The reference aqueous pressure is 12.3 MPa at the reference depth of -1041 m; the reference temperature is 35.9°C at the reference depth of -1001 m. The initial average temperature in the region surrounding the four wells of the reservoir is about 36°C . The Brooks and Corey parameters λ is 0.8311, aqueous residual saturation is 0.0597, and actual gas residual saturation is 0.2 according to field surveys.

Different boundary conditions are appropriate for flow boundaries and are applicable to the conservation equations for water, CO_2 , and salt mass. A zero flux boundary condition specifies an impermeable boundary for flow or transport at the bottom boundary. Initial values of aqueous pressure, temperature, and salt mass fraction in the nodes adjacent to a boundary surface were used as constant boundary conditions. Here zero flux boundary conditions were applied for the gas phase along all boundaries.

7. ABAQUS 3D model

A 3D ABAQUS[®] finite element model of the FutureGen 2.0 site that exactly maps the STOMP-CO2 model (Figure 3) was built for the coupled analysis using STOMP-CO2/ABAQUS[®]. This model contains $60 \times 60 \times 31$ 3D solid 8-node linear brick finite elements. The ABAQUS[®] modeling domain is identical to the STOMP-CO2 domain that contains 31 layers listed in Table 3. The pressure loading was applied on the top surface that captured the gravity pressure varying with the top surface depth (Figure 8). **In order to achieve the strike-slip faulting stress regime reported in Cornet (2004), measured in-situ stresses by Cornet (2004) were explored to define the stress ratios that have been used in the application of boundary conditions on the lateral surfaces of the model. Table 4 gives the lower and upper bounds of the maximum horizontal stress (σ_H) as well as the vertical stresses (σ_V) determined by Cornet (2004) at various depths from 1267 m to 1407 m. σ_T in Table 4 denotes the tensile rock strength that was assumed to be about 5.2 MPa. First, for a given depth in Table 4, an average σ_H/σ_V ratio is calculated and presented in this table. The mean of these four stress ratio values is $\sigma_H/\sigma_V = 1.331$, thus $\sigma_H = 1.331\sigma_V$ has been applied at a lateral model boundary surface as depicted in Figure 8 where the measured vertical stress can be fitted by $\sigma_V = 0.025z$ with z being the coordinate in the vertical direction. Cornet (2004) also found that the minimum horizontal principal stress σ_h does not vary linearly with depth within the Mount Simon Sandstone. Two test-derived values reported for σ_h at two different depths, 1267 m and 1291 m are 22.3 MPa**

and 19.3 MPa, respectively. However, the three measurements conducted between 1,407 m and 1,378 m in the Precambrian crystalline basement rock exhibit results consistent with a local linear increase with depth: $\sigma_h = 26.5 + 0.0212(z - 1,378)$ MPa (Cornet, 2004). Because of the difference in the observed behavior of σ_h as a function of depth, in the present analysis, zero-normal displacements were applied on all the other lateral boundary surfaces and the bottom surface of the model (Figure 9). In addition, gravity loading in the z -direction was applied inside the formation, and the fluid pressure computed by Eq. (2) using STOMP-CO2 results was prescribed at the selected times during the STOMP-CO2/ABAQUS[®] analysis. The temperature distributions provided by STOMP-CO2 were captured at the selected times, and the temperature changes were determined to compute thermal stresses in Eq. (1). Figures 9 and 10 give the values of the elastic modulus and of the coefficient of thermal expansion (CTE) for all the layers through the formation depth along a vertical direction containing the vertical portion of injection wells. These properties for the analyses were derived from geophysical well logs and the literature for 31 layers at the FutureGen 2.0 site. The median values of elastic modulus and Poisson's ratio for each layer were taken from geophysical well logs run in a characterization well drilled at the site. The CTE for a layer was estimated by a weighted average of the pure phase mineral thermal expansion coefficients, where the weights were the volume fractions of all minerals in the solid phase estimated from geophysical well logs. The Poisson ratios are in the 0.16 to 0.3 range. As previously mentioned, uniform properties were assigned to each varying-depth layer.

Table 4. Summary of expected magnitudes for the principal stress components σ_H and σ_V according to Cornet (2004).

Depth (m)	Lower bound σ_H (MPa)	Upper bound σ_H (MPa)	Assumed σ_T (MPa)	σ_V (MPa)	Average ratio σ_H/σ_V
1267	$29.62 + \sigma_T$	$42.23 + \sigma_T$	5.17	30.69	1.34
1291	$24.17 + \sigma_T$	$37.03 + \sigma_T$	5.17	31.28	1.14
1387	$32.32 + \sigma_T$	$46.13 + \sigma_T$	5.17	33.61	1.32
1407	$39.71 + \sigma_T$	$53.71 + \sigma_T$	5.17	34.08	1.52

Figure 8. The 3D finite element model with associated boundary conditions for the analysis.

Figure 9. Assigned elastic modulus for the layers in the model: A uniform value was assigned to each varying-depth layer. CO₂ is injected between depths 1191 m and 1233 m.

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Figure 10. Assigned coefficient of thermal expansion (CTE) for the layers in the model: A uniform value was assigned to each varying-depth layer. CO₂ is injected between depths 1191 m and 1233 m.

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8. Results

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The 31-layer formation (Figure 3) was subjected to CO₂ injection at temperatures 28°C and 47°C and analyzed by STOMP-CO₂/ABAQUS[®]. We have named these analysis cases as Case 28C and Case 47C, respectively. Case 47C, which corresponds to the yearly average fluid temperature predicted by CO₂Flow using a reasonable range of soil conductivities for the planned pipeline route, was considered as the *reference case*. Case 28C is the lowest injection temperature predicted by CO₂Flow during winter conditions and for a short period of time and can be considered as an end-member case. The thermo-poroelastic constitutive model implemented in ABAQUS[®] (Section 4) was used for the analyses of the above cases. The exchange of data between STOMP-CO₂ and ABAQUS[®] occurred at 48 selected times over a total period of 20 years. The time intervals were chosen considering computational demand for coupled simulations, while ensuring the time intervals were short enough to avoid dramatic changes between time steps in modified permeability and porosity.

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8.1 Verification of Predicted Initial Stresses

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Before analyzing the reservoir model including CO₂ injection, it is necessary to compare the predicted initial stresses resulting from the application of boundary and loading conditions

(before CO₂ injection) to the available measured stress data at selected locations. This verification step is important to make sure that the applied boundary and loading conditions produce a stress distribution in the formation that achieves the strike-slip faulting regime observed at the FutureGen 2.0 site. Figure 11(a) shows a vertical zoom-in section of the mesh passing through the wells region where we examine the initial principal stresses along a vertical path from the model bottom at $z = 1346$ m to $z=1172$ m. Figure 11(b) reports the initial principal stresses along this path. In terms of magnitude, the minimum (σ_h) and maximum (σ_H) horizontal stresses correspond to σ_{xx} and σ_{yy} , respectively. The vertical stress (σ_v) is σ_{zz} . Figure 11(b) clearly shows that $\sigma_h < \sigma_v < \sigma_H$ as observed through the in-situ stress measurements (Cornet, 2004). In addition, for the selected depths in Table 4, the predicted maximum horizontal stresses are within the lower and upper bounds. The predicted vertical stress σ_v is a nearly linear function of depth and also is in good agreement with the corresponding estimated values from Cornet (2004). The predicted minimum horizontal stress values within the Mount Simon sandstone at depths 1267 m and 1291 m are 21.8 MPa and 23.1 MPa, respectively compare fairly well with the measured values (i.e., 23.3 MPa at 1267 m and 19.3 MPa at 1291 m). Figure 12 gives the stress ratios resulting from the initial principal stresses along the selected path. This figure and Figure 11 confirms the strike-slip faulting stress regime found in Cornet (2004).

Figure 11. (a) A vertical zoom-in section of the mesh passing through the wells region where a vertical path from the model bottom from $z = 1168$ m to $z = 1341$ m was defined to examine the initial principal stresses, (b) Predicted initial principal stress components along this path.

Figure 12. Predicted stress ratios along the vertical path defined on Figure 11(a).

8.2 Analysis of Case 47C

Figure 13 provides the two-dimensional (2D) view of the injection well # 1 (Figure 13a), the evolutions of temperature (Figure 13b), fluid pressure (Figure 13c), pressure margin to fracture (PMF) (Figure 13d), and strength-to-stress margin (SSM) (Figure 13e) versus time for this well at the selected locations for Case 47C, the reference case. In this well and also in the other horizontal wells, four representative locations at different depths were selected for illustrating the evolutions of the above variables. The injection temperature was 47°C. The temperature distributions predicted by STOMP-CO2 at the selected locations on Well # 1 illustrated in Figure 13b show an increase in temperature for all the nodes of the well. In particular, Location numbered 30635 experienced an increase in temperature of about ~4°C after 20 years. An increase in temperature renders the principal effective stresses (given in Eq. (6)) more compressive, and as a consequence, enlarges the pressure margin to fracture. Therefore, PMF did not exceed zero at any node and time step for this case but exhibited a trend to enlarge with the increase of temperature as clearly shown in Figure 13d that reports the evolution of PMF vs. time at the selected locations on Well # 1. The predicted fluid pressure versus time for the same locations given in Figure 13c rapidly evolved and stabilized at about 15.5 MPa after two years. The strength-to-stress margin SSM for shear slip activation evaluated for these locations using Eq. (10) are reported in Figure 13e which shows a trend to increase with the increase of temperature except for the first several months that experienced slight reductions in SSM due to a rapid increase in fluid pressure. However, as time went on, the fluid pressure stabilized (Figure 13c), and the increase in temperature then increased the SSM along the well. Similar results and

findings were found for three other wells for this case. Thus, injecting CO₂ at 47°C would not cause hydraulic fracture or shear slip failure of the reservoir.

Figure 13. (a) 2D view of Well # 1, (b) temperature evolution, (c) pressure evolution, (d) PMF evolution, and (e) SSM evolution for the selected locations on Well # 1 (Case 47C).

8.3 Analysis of Case 28C

For this case, the injection temperature was 28°C which can be considered as an extreme low temperature case since it corresponds to winter conditions maintained throughout the year which is very unlikely to happen. The temperature distributions predicted by STOMP-CO₂ at some of the selected locations on four wells showed a global decrease in temperature. In particular, locations numbered 30635 on Well # 1 (Figure 14b), 30213 on Well # 2 (Figure 15b), 30267 on Well # 3 (Figure 16b), and 30566 on Well # 4 (Figure 17b) experienced a decrease in temperature about ~3°C at 20 years. We also observed slight increases in temperature at some locations during the first year of injection due to the exothermic dissolution of CO₂ into the brine water. The temperature increases that involve the heat of CO₂ dissolution into water is well understood as an exothermic reaction in the three-dimensional region partially filled with CO₂ as the pressure wave moves outward over time (Han et al., 2010). The resulting heat can dissipate out at the ends of the wells, but not as quickly closer to the middle of the high pressure bubble, which is influenced more by all four wells. When time goes on, the heat transfer resulting from lower injection temperature then brings the temperatures down.

The fluid pressure evolutions (Figures 14c to 17c) are similar to those for Case 47C. They rapidly evolved and stabilized at about 15.5 MPa after two years. The decrease in temperature observed in Case 28C renders the principal effective stresses (Eq. 6) less compressive, and as a consequence, reduces the pressure margin to fracture PMF. Since the pressure evolution in Case 28C was rapid and matched that of Case 47C, the reduction of PMF was caused by the decrease in temperature at some examined locations due to the lower injection temperature (compared to Case 47C). However, the hydraulic fracture criterion was not exceeded along any wells. Figures 14d, 15d, 16d and 17d show that the reduction of PMF was more significant for Locations 30635, 30213, 30267, and 30566 on Wells # 1, 2, 3, and 4, respectively. These locations first experienced a slight increase in temperature due to the exothermic CO₂ dissolution effect during the first months of injection. The heat transfer due to lower injection temperature then decreased the temperatures at these locations leading to the reduction of PMF. The progressive decrease in temperature from 36.6°C at two years to 35.7°C at 20 years caused the PMF at Locations 37832 (on Well # 1) and 37769 (on Well # 4) to decrease. The evolutions of temperature and PMF at Location 34111 on Well # 2 (Figures 15b and 15d) and at Location 34110 on Well # 3 (Figure 16b and 16d) exhibited similar trends to those at Locations 37832 on Well # 1 and Location 37769 on Well # 4, however, the decreases in temperature were smaller, and as a result, the reduction in PMF were very small at these locations. The other locations numbered 59431 on Well # 1, 59371 on Well # 2, 59370 on Well # 3 and Well # 4 exhibited very small temperature changes, and therefore, the PMF at these locations underwent minor variations after an initial reduction at up to two years caused by the increase in injection pressure.

The strength-to-stress margin SSM given by Eq. (10) was used to predict shear slip activation along these four wells, and the SSM results are reported in Figures 14e, 15e, 16e and 17e for Wells # 1, 2, 3, and 4, respectively. Before the start of the injection, SSM was globally positive

along the four wells except Locations 37832 (Well # 1), 44971 (Well #2), 44970 (Well # 3), and 37769 (Well # 4) exhibited slightly negative values of SSM. A very small increase in temperature due to the exothermic CO₂ dissolution effect during the first months of injection has slightly increased SSM in these locations. However, as time went on, the decrease in temperature at these locations rendered the SSM more and more negative. Therefore, shear slip activation was predicted to occur in all four wells after about 5 years of CO₂ injection. As discussed in Vilarrassa et al. (2013), the effect of shear slip can be advantageous when it occurs within the reservoir aquifer as it enhances the reservoir permeability, thus increases CO₂ injectivity. It is therefore important to examine the extent of shear slip activation and other potential fracture due to the thermal effect. In order to assess the extent of the predicted fracture area and the effect of temperature drop, Figure 18 presents the temperature distribution at 20 years through a cross section perpendicular to the x -axis at $x = 237368$ m and passing through the wells region. A zoom-in of the wells region is also shown in Figure 18 to assess the area impacted by the temperature drop.

Next, Figures 19 and 20 show the temperature and PMF contours at the beginning of the injection (year 0) and year 20 of injection for the same section and region. These results show that the PMF was reduced at 20 years in the wells region (Figure 19a vs. Figure 20a) but only locally and was still negative and below the margin at fracture. The reduction of PMF was caused by a temperature drop as clearly shown in Figures 19b and 20b for the temperature distributions. Figures 21a and 21b present the strength-to-stress margin SSM contours at the beginning (year 0) and at 20 years, respectively. The thermal effect due to 20-year CO₂ injection at 28°C is clearly observed in Figure 21b that shows locally negative values of SSM along the wells. So, local shear slip activation was predicted to occur in the wells region in Case 28C. As indicated in Figure 21b, shear slip activation has been found to remain between MtSimon4_5 and MtSimon17, so it was predicted to occur within the Mount Simon reservoir (Figure 1). In this case, shear slip activation would not be a concern.

Figure 14. (a) 2D view of Well # 1, (b) temperature evolution, (c) pressure evolution, (d) PMF evolution, and (e) SSM evolution for the selected locations on Well # 1 (Case 28C).

Figure 15. (a) 2D view of Well # 2, (b) temperature evolution, (c) pressure evolution, (d) PMF evolution, and (e) SSM evolution for the selected locations on Well # 2 (Case 28C).

Figure 16. (a) 2D view of Well # 3, (b) temperature evolution, (c) pressure evolution, (d) PMF, and (d) SSM evolution for the selected locations on Well # 3 (Case 28C).

Figure 17. (a) 2D view of Well # 3, (b) temperature evolution, (c) pressure evolution, (d) PMF, and (d) SSM evolution for the selected locations on Well # 4 (Case 28C).

Figure 18. Vertical cross section perpendicular to the x -axis and passing through the region of the wells showing the predicted temperature distribution at 20 years – A zoom-in of the wells is also illustrated. The dimensions in the Z-direction (vertical direction) were amplified 100 times.

Figure 19. The initial PMF (a) and temperature (b) distributions (Case 28C) in the region of the wells. For visualization of results, the vertical coordinates (z-direction) were amplified 100 times.

Figure 20. PMF (a) and temperature (b) distributions (Case 28C) in the region of the wells at 20 years.

Figure 21. (a) The initial SSM contour, and (b) SSM contour at 20 years in a vertical view showing the region of the wells (Case 28C).

To further illustrate the change in stress distributions from Year 0 to Year 20 as a result of the injected CO₂ at 28°C, Figures 22(b-d) report all the principal effective stress components along the vertical path (shown in Figure 22a) passing through the wells region from $z = 1168$ m to $z = 1341$ m. These figures clearly show that all the stress components were initially compressive and well below the margin at hydraulic fracture. However, after 20 years of CO₂ injection at 28°C, σ'_{xx} , σ'_{yy} and σ'_{zz} have all increased (less negative) significantly in the well region (between 1191 m and 1250 m).

Figure 22. (a) The vertical path defined and shown in Fig. 11a, (b) Principal effective stress σ'_{xx} (c) Principal effective stress σ'_{yy} , and (d) Principal effective stress σ'_{zz} at the beginning and at 20 years along this path.

8.4 Deformation of the model top surface

Due to underground CO₂ injection that induces stress and strain redistributions in the reservoir, the ground surface at the storage site undergoes deformation that evolves with time with respect to its initial position. To have an estimate of the ground surface deformation, we examined the vertical displacements of the formation model computed by STOMP-CO₂/ABAQUS[®] analyses. The contours of the vertical displacements predicted at 20 years for Cases 47C and 28C are given in Figures 23 and 24 that show the views through a vertical section perpendicular to the *x*-axis at Well # 1. These figures clearly indicate the maximum value occurring immediately above the wells. **The peak of the vertical displacement at 20 years for Case 47C is about 0.023 m, and it is about 0.018 m for Case 28C.** Figure 25 provides the evolutions of the maximum vertical displacement on the top surface of the model as a function of time for both cases. The maximum vertical displacements illustrated in Figure 25 increased quickly from year 0 to about year 2 and progressively slowed down after 2 years. These evolutions have a somewhat similar trend as the fluid pressure vs. time evolution at the wells. Therefore, they were controlled by the fluid pressure in the wells region in addition to the temperature effect that is also observed in Figure 25. Compared to the solutions predicted for Case 47C, lower CO₂ injection temperature rendered the effective principal stresses less compressive around the wells but affected the deformation for the top layers due to a multilayer effect and led to lower maximum vertical displacement for Case 28C.

Figure 23. Contour of vertical displacements predicted at 20 years for Case 47C.

Figure 24. Contour of vertical displacements predicted at 20 years for Case 28C.

Figure 25. Evolution of the maximum vertical displacement on the top surface vs. time predicted for Cases 47C and 28C.

9. Discussion

9.1 Assessment of the STOMP-CO2/ABAQUS[®] solution with the data update frequency

The sequentially coupled approach can provide as accurate solutions as the fully coupled approach if the frequency for the data update (exchange) between the flow sub-problem and geomechanical sub-problem is very fine. However, to avoid prohibitively high numbers of required steps, it is important to assess the convergence of the sequentially coupled solution with the refinement of the frequency for the data update. This assessment is illustrated in Figures 26a for the temperature, Figure 26b for the fluid pressure, and Figure 26c for the PMF for Case 28C, in Well # 1 at Location 30635. In Scenario 1 for the data update (that was actually used in the analyses), STOMP-CO2 provides the needed variables to ABAQUS for geomechanical analysis according to computational procedure depicted in Figure 2, and receives updated values for the selected variables occurs respectively at 1 day, every 30 days during 1 year, every 60 days during 2 years, every 180 days during 3 years, every 240 days during 4 years, and every year until completing the 10 year-period of CO₂ injection. In Scenario 2, the update/exchange data between STOMP-CO2 and ABAQUS occurs at 1 day and then regularly every 30 days. Figures 26(a-c) show that the results are in excellent agreement, and Scenario 1 with a coarser exchange data frequency can accurately capture the solution based on a much finer frequency of data update. The predicted fluid pressure and stress levels were moderate resulting in very small changes in porosity and permeability. The maximum changes in porosity and permeability occurred during the analysis were about 0.2% and 1.07%, respectively. We also note that the reservoir layers (Layers MtSimon 11 to MtSimon17) are generally very stiff and some possess elastic modulus higher than 50 GPa leading to very small strains under moderate stresses and fluid pressures. The very small changes in permeability and porosity justified the coarse frequency of exchange data between STOMP-CO2 and ABAQUS[®].

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722 **Figure 26. Sensitivity study of the frequency for data exchange and update between STOMP-**
 723 **CO2-R and ABAQUS®.**

724 9.2 Temperature distribution and effect of injection temperature

725 STOMP-CO2's thermal solution for the temperature distribution evolution in the FutureGen
 726 2.0 site's model was obtained using the grid presented in Figure 3a. This grid contains fine
 727 discretizations for the reservoir layers and in particular the region involving the four wells. In
 728 this region the sizes of the cells in the X and Y directions are 152 m x 150 m while the varying
 729 thicknesses of the elements can be found in Table 3. In the pre-design stage of the FutureGen 2.0
 730 site, these discretizations along X and Y are very fine with respect to the X - Y dimensions of the
 731 whole domain (~166000 m x ~166000 m) and are sufficient to capture the thermal impact of CO₂
 732 injection on the geomechanical response of the site. In fact, further refinement of the grid in the
 733 region of the wells and adjacent areas would produce a temperature around the injection wells
 734 closer to the injection temperature as Gor et al. (2013) found in their problem using a much finer
 735 2D mesh. The analyses of the FutureGen 2.0 site using finer 3D grids would not significantly

alter the findings based on the actual analyses using the grid given in Figure 3a because the temperatures in the more finely discretized well region would be closer to the injection temperature and would render the PMF more compressive and increase SSM in the examined locations in Case 47C and would also exacerbate the exceedance of the shear slip activation criterion in Case 28C.

9.3 Estimate of the ground surface deformation

Our model does not include the ground surface. The estimate of the ground surface vertical displacement can be only a rough approximation. To estimate the likely order of magnitude of the maximum vertical displacement on the ground surface, we have plotted in Figure 27 for both cases the maximum vertical displacements at 20 years along a vertical path from the bottom to the top model surface passing through the wells and inside the maximum vertical displacement zones (Figures 23 and 24). Figure 27 clearly shows that in both cases the maximum vertical displacements increase from the model bottom and reach the maximum values and have a trend to lightly decrease until reaching the top surface. Because the injection pressure is constant after 2 years of injection (about 15.5 MPa) and the thermal effect decreases near the ground surface, this trend suggests that the maximum displacements on the ground surface would be less than 0.025 m for Case 47C and less than 0.018 m for Case 28C. It is also expected that for injection temperatures between 28°C and 47°C the maximum displacements on the ground surface would occur at the location right above the wells and would be less than 0.025 m.

Figure 27. Maximum vertical displacements from the model bottom to the model top computed for Case 47C and Case 28C.

10. Conclusions

An evaluation of the potential thermal impact of CO₂ injection on the FutureGen 2.0 site was performed using the STOMP-CO2 code sequentially coupled to the ABAQUS[®] finite element package. Based on the results from hydraulic modeling of CO₂ flow in pipelines and injection wells, two injection temperature cases were analyzed by the STOMP-CO2/ABAQUS[®] simulator: 28°C and 47°C. The STOMP-CO2 and ABAQUS[®] models built for the analyses were fully three-dimensional with four horizontal wells and variable layer thickness. The measured in-situ stresses at selected depths from Cornet (2014) were explored to determine the geomechanical boundary conditions to achieve the strike-slip faulting stress regime observed at the FutureGen 2.0 site. The predicted initial stresses in the formation were found to reasonably agree with the measured stresses at the selected locations and capture the observed stress regime.

Thermally induced hydraulic fracturing is not predicted to occur for any injection temperatures. However, shear slip activation is predicted to occur for injection temperatures approaching 28°C which can be considered as an extreme low and unlikely temperature case since it corresponds to winter conditions maintained throughout the year. Injection temperatures in that range would lower the reservoir temperature near the wellbore by ~3°C after 20 years for an injection temperature of 28°C. Shear slip would occur at critical locations after about five years of injection (given the conservative criterion used). Nevertheless, the zones where the strength-to-stress margin SSM would exceed the shear slip activation criterion for 28°C injection temperature were found adjacent to the wellbore and nearby locations between MtSimon4_5 and MtSimon17. Even if shear slip activation would occur under these extreme conditions, it would be limited to occur close to injection wells and would therefore not jeopardize the confinement of the CO₂, but on the other hand could increase injectivity.

The geomechanical evaluation of thermal stresses performed for this study indicates that failure of the reservoir rock due to thermally induced hydraulic fracturing and shear slip are not predicted to occur for injection temperatures of 47°C or higher which represents the annual average injection temperature. In that temperature range, the injection temperature would be at or above the natural reservoir temperature. Increasing the temperature of the reservoir by CO₂ injection would render the principal effective stresses more compressive, and as a consequence, enlarge the pressure margin to fracture and strength-to-stress margin making it even less likely to fracture. Based on the results of this study and the expected range of injection temperatures for CO₂ at FutureGen 2.0, thermally induced fracturing is not predicted to occur.

Acknowledgements

This material is based upon work supported by the Department of Energy under Award Number DE-FE0001882 and Award Number DE-FE0005054. The authors would like to thank Dr. Jonny Rutqvist, Staff Scientist at Lawrence Berkeley National Laboratory, two anonymous reviewers and the Associate Editor, Dr. Jens Birkholzer for their detailed reviews that have

contributed to greatly improve this manuscript. The authors also thank Dr. Fred Zhang and Ms. Signe White, Senior Research Scientists at Pacific Northwest National Laboratory for their assistance in developing the STOMP-CO₂ model and for helpful discussions. STOMP-CO₂/ABAQUS[®] analyses were performed using PNNL Institutional Computing at Pacific Northwest National Laboratory.

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Appendix

931 **Table A1.** Major material properties for the aggregate layers: Young's modulus E (GPa), Poisson's
 932 Ratio ν , porosity, thermal expansion coefficient β ($10^{-5}/^{\circ}\text{C}$), permeability components k_{xx} , k_{yy} , k_{zz} , and
 933 norm k (m^2), and capillary entry pressure P_c (m).

Aggregate Layer	E	ν	β	Porosity	$k_{xx}=k_{yy}$	k_{zz}	k	P_c
Franconia	84.98	0.279	3.156	0.0358	5.43E-21	3.80E-23	1.04E-21	234.426
Davis-Ironton	61.73	0.272	2.921	0.0317	4.14E-15	9.25E-18	5.41E-16	2.818
Ironton-Galesville	45.99	0.227	4.643	0.0981	2.60E-14	1.04E-14	1.91E-14	1.076
Proviso4_5	36.38	0.306	2.648	0.0813	1.82E-18	1.27E-19	7.49E-19	40.255
Proviso1_3	54.94	0.294	2.637	0.0502	4.26E-17	8.51E-21	2.49E-18	11.516
Lombard12_14	37.93	0.291	2.682	0.1044	9.65E-17	1.42E-19	1.10E-17	10.266
Lombard8_11	39.23	0.266	3.427	0.0753	4.26E-15	2.33E-18	3.49E-16	2.788
Lombard5_7	48.4	0.248	4.161	0.0696	1.78E-13	3.32E-15	4.71E-14	0.773
Lombard1_4	43.6	0.252	3.419	0.0762	1.49E-15	9.75E-18	2.79E-16	4.004
Elmhurst7	38.56	0.207	4.245	0.1595	2.01E-14	8.06E-15	1.48E-14	1.182
Elmhurst6	32.68	0.239	3.965	0.1981	1.82E-13	7.28E-14	1.34E-13	0.525
Elmhurst5	42.13	0.225	3.845	0.0822	1.85E-15	1.85E-16	8.57E-16	3.718
Elmhurst4	46.82	0.187	4.332	0.1105	4.91E-15	1.96E-15	3.62E-15	1.991
Elmhurst3	45.55	0.253	3.69	0.0768	7.42E-16	7.42E-17	3.45E-16	5.09
Elmhurst2	43.77	0.223	4.311	0.1291	1.61E-14	6.45E-15	1.19E-14	1.284
Elmhurst1	41.36	0.238	3.707	0.083	2.86E-16	2.86E-17	1.33E-16	7.064
MtSimon17	43.25	0.215	4.618	0.1297	7.17E-15	2.87E-15	5.28E-15	1.732
MtSimon16	45.78	0.221	4.437	0.1084	3.73E-16	3.73E-17	1.73E-16	6.447
MtSimon15	48.26	0.185	4.644	0.1276	5.01E-15	2.00E-15	3.69E-15	1.975
MtSimon14	51.5	0.199	4.739	0.1082	1.31E-15	5.26E-16	9.68E-16	3.236
MtSimon13	50.06	0.189	4.661	0.1278	5.26E-15	2.10E-15	3.88E-15	1.941
MtSimon12	42.98	0.22	4.506	0.1473	1.57E-14	6.26E-15	1.16E-14	1.298
MtSimon11	26.16	0.269	4.588	0.2042	3.06E-13	1.53E-13	2.43E-13	0.434
MtSimon10	43.66	0.192	4.59	0.1434	1.37E-14	4.13E-15	9.19E-15	1.362
MtSimon9	43.46	0.186	4.614	0.1434	1.37E-14	4.13E-15	9.19E-15	1.362
MtSimon8	45.6	0.179	4.748	0.1503	2.07E-14	6.21E-15	1.39E-14	1.171
MtSimon7	47.11	0.17	4.704	0.1311	6.43E-15	1.93E-15	4.30E-15	1.803
MtSimon6	48.9	0.165	4.578	0.1052	2.23E-15	6.69E-16	1.49E-15	2.664
MtSimon4_5	37.73	0.208	4.065	0.1025	5.80E-15	1.68E-16	1.78E-15	1.872
MtSimon2_3	36.01	0.235	4.092	0.0506	2.54E-15	7.42E-16	1.68E-15	2.541
MtSimon1	35.6	0.244	3.526	0.1157	2.83E-15	2.83E-16	1.32E-15	2.439

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