Evaluating the impact of aquifer layer properties on geomechanical response during CO₂ geological sequestration

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A B S T R A C T

Numerical models play an essential role in understanding the facts of carbon dioxide (CO₂) geological sequestration in the life cycle of a storage reservoir. We present a series of test cases that reflect a broad and realistic range of aquifer reservoir properties to systematically evaluate and compare the impacts on the geomechanical response to CO₂ injection. In this study, a coupled hydro-mechanical model was applied to simulate the sequestration process, and a quasi-Monte Carlo sampling method was employed to efficiently sample the value of aquifer properties and geometry parameters. Through quantitative sensitivity analysis, the impacts of all the input parameters are ranked. Aquifer permeability was found to be of significant importance to the geomechanical response to the injection. To study the influence of uncertainty of the permeability distribution in the aquifer, an additional series of tests is presented, based on a default permeability distribution site sample with various distribution deviations generated by the Monte Carlo sampling method. The results of the test series show that the uncertainty of permeability distributions significantly affect the displacement and possible failure zone.

1. Introduction

Injecting fluid into confined aquifers is a widely accepted strategy for enhanced oil recovery, gas storage, and waste disposal (Nordbotten and Celia, 2006). It is well known that carbon dioxide (CO₂) sequestration in deep saline aquifers could be a promising mitigation method for the reduction of CO₂ emitted to the atmosphere (Vilarrasa et al., 2011). The storage of CO₂ in deep saline aquifer is an excellent solution for large parts of northwest Europe and the midwestern United States, where large-scale CO₂ storage will be required in order to make a significant contribution to reduce CO₂ emissions (Rutqvist et al., 2010). Geological storage of CO₂ involves fairly complex physical and chemical processes such as multiphase flow, multicomponent miscible transport, geochemical (Spycher et al., 2003), geomechanical, and nonisothermal effects (Celia and Nordbotten, 2010; Rutqvist, 2012). Mathematical models and numerical simulation tools will play an important role in evaluating the feasibility of CO₂ storage in subsurface reservoirs, designing and analyzing field tests, and designing and operating geological CO₂ disposal systems (Pruess et al., 2004). Because of the complexity of the CO₂ geological sequestration, many factors impact the safety and sustainability of the injection. This paper presents a computational model and a series of test cases for understanding the importance of different factors that affect geomechanical response upon the injection of substantial supercritical CO₂ into a deep geological formation. In addition, various aquifer permeability distributions are generated to represent different stone formations in aquifers for understanding the geomechanical response following the injection of CO₂ into various formations.

CO₂ is expected to be retained underground until well past the end of the fossil fuel era, and it could last several hundred years or even longer than 1000 years (Wilson, 1992; Holloway, 2005). Hence, geological sequestration of supercritical CO₂ intrinsically involves a number of complicated physical and chemical processes that occur within a large spatial domain and an extremely long period of time. In addition, the sensitivity analysis of input parameters requires hundreds of simulation cases. To make the simulation computationally affordable, the numerical model used for CO₂ sequestration must be stable within a large time step and grid size. The numerical model we used in all test cases is stable for time steps ranging from a day to a few years, and the grid size can be several hundred meters. The accuracy is tested through comparing with the analytical solution (Bao et al., 2012).

We first introduce and discuss the input parameter sensitivity analysis in Section 2. During CO₂ injection, the fluid pressure may...
be too large, and the induced stress may cause irreversible mechanical changes, create new fractures, and reactivate existing faults (Rutqvist et al., 2007), which may cause seismic activity. In the same section, we describe the application of geomechanical shear-slip failure analysis to estimate the potential damage zone during CO2 injection. The quasi-Monte Carlo method was applied for sampling model input parameters to achieve the balance between covering as many as possible over the entire parametric space without introducing undesired bias and computational burden, which are discussed in Section 2.2. We also discuss the uncertainty of structure of layering aquifer permeability distribution’s impact to geological displacement during CO2 sequestration in Section 3.

2. Input parameter sensitivity analysis

The sensitivity analysis of the input parameters for geomechanical response during CO2 injection was based on the simulation results of a coupled hydro-mechanical model (Xu et al., 2012). The model can be solved analytically for a simplified typical CO2 sequestration problem in the axisymmetric coordinate system, as shown in Fig. 1. A numerical solution was developed for arbitrary geometry (Bao et al., 2012) using a finite element method (FEM) code based on an open-source FEM program Elmer (CSC-IT, 2011), which shows great agreement with the analytical solution. For convenience, the model is briefly introduced in Section 2.1. The quasi-Monte Carlo is a popular sampling method because of their faster convergence and effective sampling of high-dimensional parametric space, which is briefly introduced in Section 2.2 for convenience as well.

2.1. A hydro-mechanical model for CO2 geological sequestration

Because the hydro-mechanical model was designed for estimating the CO2 geological sequestration over a long time period and in a large space domain, several assumptions were used: details in microscale and rapid transition phenomena were neglected; heat transport and geochemical reaction were considered irrelevant to the geomechanical response; and the stress and geological deformation did not significantly change the properties of fluid flow. The hydro-mechanical model included both fluid flow and linear elasticity equations that describe the geomechanical response due to the fluid injection. The coupled hydro-mechanical model (Terzaghi, 1923; Biot, 1935, 1941, 1955, 1956, 1962) reads

\[
\frac{\partial p}{\partial t} + \frac{1}{\gamma} \left( \nabla \cdot \mathbf{u} \right) = \frac{k}{\gamma \mu} \nabla^2 p + \frac{\psi}{\gamma \mu} (\lambda + 2G) \nabla (\nabla \cdot \mathbf{u}) + \nabla \cdot \nabla \mathbf{u} = \nabla p
\]  

Eq. (1) is a Darcy flow equation in terms of \( p \), which is defined as the difference between current pressure (\( p_c \)) and initial pressure (\( p_i \)), namely \( p = p_c - p_i \). In Eq. (1), \( t \) is the injection time, \( \mathbf{u} \) is the displacement vector, \( \gamma \) is the porosity, \( \mu \) is the fluid compressibility, \( k \) is the permeability, \( \rho \) is the density of liquid, and \( \psi \) is the external source term representing the CO2 injection rate with a unit of kg/(m\(^3\) s). Eq. (2) is a Navier type of elasticity equation in terms of the displacement vector \( \mathbf{u} \). In Eq. (2), \( G \) is the shear modulus and \( \lambda \) is Lane’s constant for the entire subsurface medium. Eqs. (1) and (2) are valid for arbitrary geometry and boundary conditions.

All test cases were simulated in a simplified practical CO2 geological sequestration in an axisymmetric coordinate system, as shown in Fig. 1, where \( r \) is the radial axis and \( z \) is the vertical axis. The CO2 injection well was located at \( r=0 \), and the ground surface (top surface) was at \( z=0 \). CO2 was injected into a confined aquifer formation from \( z_1 \) to \( z_2 \). The permeability of the caprock and base were assumed small enough to confine the fluid flow. Because the model is single-phase and the density is assumed to be constant, the effect of gravity is neglected. Our previous work introduced an analytical (Xu et al., 2012) and a finite element model (Bao et al., 2012) to solve this coupled system in an axisymmetric coordinate system. The boundary conditions for the proposed model

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**Fig. 1.** Simulation domain and geometry configuration.
(Eqs. (1) and (2)) are
\[ u_r = 0, \quad u_z = 0, \quad p = 0 \text{ at } r = \infty \text{ or } z = -\infty \] (3)

For finite element model, the boundary conditions are set at \( z = -40 \text{ km}, \) and \( r = 80 \text{ km} \) to mimic the boundary conditions at \( z = -\infty \) and \( r = \infty \). The displacements and pressure are all zero at time \( t = 0 \) s. The CO2 injection is a multi-phase system, while the proposed model (Eq. (1)) assumes it as single-phase. Fig. 2 shows the comparison between the results from the proposed single-phase flow model (Eqs. (1) and (2)) and the results from a CO2-brine multi-phase subsurface flow simulator, STOMP (Subsurface Transport over Multiple Phases) (White and Oostrom, 2006) in the same geometry and boundary conditions (aquifer layer is from \( z = -2240 \text{ m} \) to \( z = -2740 \text{ m} \) (Gollakota and McDonald, 2012), and injection rate is 350 kg/s (Hitchon, 1996)). Although single-phase model slightly overestimates the pressure than the multi-phase model (STOMP) simulation near the injection well, the proposed model can catch the character of the pressure evolution in aquifer, because pressure evolution is much faster than flow transport. Therefore, the proposed single-phase flow model is an efficient tool to estimate the geomechanical response to the CO2 injection practices, especially for the uncertainty quantification.

The maximum pressure (pressure at the injection well, as indicated in Fig. 2), an important parameter that reflects the safety and sustainability of the injection well, was selected for sensitivity analysis. Fig. 3(a) and (b) shows the analytical and FEM results for radial and vertical displacements at the top surface. The maximum radial and vertical displacements at the top surface, indicated in Fig. 3, were another two model outputs selected for sensitivity analysis. Top surface/ground surface displacements are critical parameters that can be used to monitor the potential hazard caused by CO2 sequestration activities. Colesanti and Wasowski’s work (Colesanti and Wasowski, 2004) shows that about 10 mm/year ground surface movement velocity can induce severe buildings’ damage in high probability. Besides that, in the practical site, the ground surface displacements are easily monitored by Global Positioning System (GPS) or satellite-borne Synthetic Aperture Radar (SAR).

Shear-slip analysis has been performed by several researchers using the magnitude and orientation of principal stresses with respect to pre-existing fault planes and fluid pressure within the fault plane (Morris et al., 1996; Wiprut and Zodack, 2000; Streit and Hills, 2004; Rutqvist et al., 2007). In our work, we applied the shear-slip analysis proposed in Rutqvist’s work (Rutqvist et al., 2007) to determine the potential failure zone. In our analysis, the cohesion was set to zero and the friction angle was 30° (Rutqvist et al., 2007; Vilarrasa et al., 2011). Thus, the criterion for shear-slip was \( |BC| \geq |BC| \) on a Mohr’s circle, as shown in Fig. 4. The failure criterion in terms of the effective principal stress was
\[
\frac{\sigma_1' + \sigma_3'}{2} - \frac{\sigma_3'}{2} \geq \sin30\circ \left( \frac{\sigma_1' + \sigma_3'}{2} \right) \rightarrow \sigma_1' \geq 3\sigma_3'
\] (4)

where \( \sigma_1' \) is the maximum effective principal stress and \( \sigma_3' \) is the minimum effective principal stress. The effective stress is calculated by
\[
\sigma' = \sigma - \rho g z
\] (5)

where \( \sigma \) is the total stress tensor and \( T \) is unit matrix. Remote stresses were applied at the model boundary in all simulations, as shown in Fig. 5. The vertical remote stress is the lithostatic stress \( \sigma_v = \rho g z \), where \( \rho \) is the density of the subsurface medium, \( g \) is
gravity, and $|z|$ is depth. Horizontal remote stress ($\sigma_h$) varies with different subsurface formations and locations. Generally, small $\sigma_h$ may cause tensile failure in higher possibility instead of shear-slip failure. $\sigma_h = 1.5\sigma_v$ (Rutqvist et al., 2007) is used in all the simulation tests in this paper, and it is a relatively big horizontal remote stress that easier leads to shear-slip failure. The indicated area is the zone in which $\Phi > 0$, namely the potential shear-slip failure zone. The maximum value of $\Phi$ also was selected as the output parameter. The value of $\Phi$ is related to the likelihood of the failure occurrence. In our study, the potential failure zone locates in the aquifer layer in the most cases, and the failure can enhance the injectivity because the fault increases the porosity and permeability of the aquifer formation (Flekkoy et al., 2002). However, frequent or continuous failure possibly causes considerable seismic activity, which may lead to ground building or facility damage. Although some pioneers paid attention to the CO2 sequestration induced seismic activity (Rutqvist, 2012), the detailed and quantitative study is still very limited, and its damage also varies a lot because of the different location and resident population. Therefore, necessary attention should be paid to the failure zone in aquifer to avoid considerable ground surface damage, though it probability enhance the injectivity.

2.2. Quasi-Monte Carlo sampling approach

Various parameters and coefficients can be adjusted in this coupled hydro-mechanical model. Among these parameters, the aquifer permeability ($k$), porosity ($\theta$), and Young’s modulus ($E = G(3\lambda + 2G)/(\lambda + G)$) were selected as the input parameters for sensitivity analysis because they can be changed over a relatively wide range for different CO2 injection sites. The Poisson ratio varies for different subsurface formation, but its impact to the geomechanical is limited in our proposed model, so it is assumed to be a fixed value 0.25. Other model parameters—for example, the viscosity ($\mu$), fluid density ($\rho$), and fluid compressibility ($\beta$)—affect the simulation results as well, but the parameter range is very limited for the practical injection. Values of these parameters were $\mu = 1 \times 10^{-3}$ Pa·s, $\rho = 600$ kg/m$^3$, and $\beta = 1 \times 10^{-6}$ (Xu et al., 2012).

In addition to the variations in property parameters, the aquifer thickness and injection well radius may be very different for various aquifer formations and injection configurations. Therefore, these two geometry parameters, as indicated in Fig. 1, were chosen as the input parameters for the sensitivity analysis. The five input parameters were selected for studying the impacts of different factors that affect the pressure, geomechanical response, and potential fracture zone during CO2 geological sequestration.

Table 1 lists the range for each of these input parameters. Young’s modulus of the stone formation that exists in aquifer, caprock, baserock, and upper varies in big range from a few GPa to over 30 GPa (Hart and Wang, 1995; Palmstrom and Singh, 2001). The entire computational domain is assumed to have the same Young’s modulus, so a small Young’s modulus may cause large displacement in the proposed model, which is not allowed in the practical cases. Therefore, the range of Young’s modulus is set as 25–35 GPa, to make the geological deformation in the desired range, such as the maximum ground surface vertical displacement smaller than 0.4 m. Similar as Young’s modulus, the aquifer porosity and permeability also vary in big range for different formation (Hou et al., 2012), but only sub-range of these two parameters are used for controlling the displacement under the acceptable range during 10 years injection. In all simulation cases, the top boundary of the aquifer was fixed at a depth of $-2242$ m, which is according to the subsurface environment for Illinois Basin-Decatur Project (Gollakota and McDonald, 2012). The permeabilities of the caprock, upper rock, and base rock were set to zero so that injected CO2 could be completely confined within the aquifer.

<table>
<thead>
<tr>
<th>Table 1</th>
<th>Input parameters and range for sensitivity analysis</th>
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<tbody>
<tr>
<td>Well radius (m)</td>
<td>0.1–0.75</td>
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<tr>
<td>Aquifer thickness (m)</td>
<td>100–500</td>
</tr>
<tr>
<td>Aquifer porosity</td>
<td>0.05–0.3</td>
</tr>
<tr>
<td>Log 10 Aquifer permeability (m$^2$)</td>
<td>–14–12</td>
</tr>
<tr>
<td>Young’s modulus (GPa)</td>
<td>25–35</td>
</tr>
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Samples should be generated to consider as much variation as possible within the parametric space without introducing undesired bias. However, as the model’s dimensionality increases, the number of samples required for a systematic approach to adequately cover the parametric space becomes unreasonable, and random or pseudorandom methods must be incorporated. Quasi-Monte Carlo methods have become increasingly popular over the last two decades because of their faster convergence and effective sampling of high-dimensional parametric space without clumping (Tarantola, 2005; Hou et al., 2012). The number of quasi-Monte Carlo samples is normally a power of 2 and is usually chosen as a trade-off between computational time and numerical error. For developing reliable responses between output and input parameters, we found that for the five-dimensional parameter space, 256 samples were adequate to yield a reliable analysis. The paired scatterplot of the five independent parameters is shown in Fig. 7, in which the sampling points in the five-dimensional parameter space are projected to a paired two-dimensional parameter plane.

2.3. Results

As mentioned in Section 2.2, five input parameters were selected for studying their impacts in CO2 geological sequestration, and four output parameters from numerical simulations were chosen to represent the mechanical response after 10 years.

Fig. 7. Paired scatterplots of the five independent input parameters.
of injection. The injection rate was fixed at 350 kg/s, which is about 11 MMT/year (Hitchon, 1996). From 256 test cases, the significance of each input was investigated through boxplots (Tukey, 1977; Benjamini, 1988; Rousseeuw et al., 1999) that show the relationship between input and output parameters (Fig. 8). Aquifer permeability clearly demonstrated the largest effect on all four output parameters, as shown by the strong linear relationship evident in Fig. 8 (column 4). The injection pressure increased with decreasing permeability, indicating that a lower injection rate should be used for a low-permeability aquifer. A lower aquifer permeability also leads to larger displacement and a larger value of \( \Phi \); that is, injecting CO\(_2\) into a low-permeability aquifer leads to larger geomechanical deformation and higher risk of failure. Aquifer thickness shows a linear relationship with maximum pressure, which is consistent with the analytical solution for pressure injection rate \( c_0 \) (kg/m s). With increasing aquifer thickness, the injection rate decreases linearly. Besides the predictable most important factor, aquifer permeability, the relative significance of the other four input parameters was not so easily determined through boxplot or analyzing the analytical solution (Xu et al., 2012) of the proposed model.

To quantitatively evaluate the sensitivity of each input parameter with respect to output variables, we employed generalized cross-validation (GCV) based on the multivariate adaptive regression splines (MARS) method (Friedman and Silverman, 1987; Friedman et al., 1988; Friedman 1991a,1991b, 1993), and standardized regression coefficients (SRCs) based on the quadratic polynomial regression method (Allison, 1977; Aiken and West, 1991; Bring, 1994) to analyze the importance and identify the sensitivity of each input parameter. Fig. 9 shows the score of importance measured by GCV and SRCs and the rank of input parameters for different output. The most important parameter, permeability, is set to a score of 100, and the scores of other inputs are scaled according to the permeability score. Both analysis methods exhibit the same rank of importance of all input parameters, which is in agreement with the qualitative conclusion obtained from Fig. 8. Aquifer thickness was the second most important factor affecting the maximum pressure and maximum value of \( \Phi \). Aquifer porosity was found to be the second most important factor affecting the top surface displacement, and Young’s modulus is ranked third. The regression and importance measurements were performed using software R (Venables et al., 2012) and PSUADE (Tong, 2010).

3. Impact of structure of layering aquifer permeability

As discussed in the previous section, aquifer permeability plays a very important role in injection pressure and geomechanical response during CO\(_2\) sequestration. In reality, the permeability
changes in an aquifer along the depth (Barnes et al., 2009; Zhou et al., 2010), as shown by the red line in Fig. 10; this was used as the default permeability distribution, which is based on the sample in Illinois Basin-Decatur Project (Gollakota and McDonald, 2012). The aquifer was divided into 53 layers, each with a different permeability value. The actual permeability distribution might differ from the sample distribution for different CO2 sequestration sites, depending on the subsurface formation. Therefore, we assume that the measured permeability from the sample is the medium value in each layer, and the actual permeability in the practical site in realistic underground environment can vary from the sample following lognormal distribution (Satter et al., 2007). To emulate this permeability distribution, the permeability in the aquifer was defined as

\[ k_i = k_{d,i} \times e^{a\chi w_i} \]  \hspace{1cm} (6)

where \( k_{d,i} \) is the permeability from the default distribution as indicated by the red line in Fig. 10 and \( i \) represents the \( i \)-th layer between 1 and 53, \( a \) is a coefficient that controls the extent of the deviation from the default permeability distribution. \( \chi \) is a 53-dimensional space used for emulating the uncertainty of 53
aquifer layers. For each value, Monte Carlo sampling was used to generate 200 samples from \( w \), which is sampled from a uniform distribution from \(-3\) to \(3\). The gray lines in Fig. 10 show 200 different permeability distributions for \( \alpha = 1 \).

The weight coefficients of bias \( \alpha \) were set to 0.2, 0.6, and 1.0. The investigation of impacts of structure of layering aquifer permeability was based on the simulation results from the numerical model introduced in Section 2.1. For Fig. 11, the radial and vertical displacements on the top surface for 200 different permeability distributions. The red line in Fig. 11 is the mean radial and vertical displacements on the top surface for 200 test cases. Figs. 12 and 13 show the mean, standard deviation, maximum, and minimum of vertical and horizontal displacements at the top surface for all 200 test cases with \( \alpha = 0.2, 0.6 \) and 1.0. It is obvious that a larger \( \alpha \) leads to larger variation of both displacements. The results show all the possible displacements, such as the best and the worst cases, based on a measured site sample with uncertain error or bias underground. It is helpful for evaluating the impact of the CO\(_2\) sequestration accurately, especially the safety of building and facility on ground surface. Figs. 14–16 show the accumulated shear-slip failure zone for the test cases. The value is scaled from 0 to 200 in Figs. 14–16. The position with the value of 200 means the shear-slip failure occurs at this position for all 200 test cases. Location with value 0 means no failure occurs in any of these 200 test cases. It can be considered as the probability of the shear-slip failure at each point in aquifer and caprock based on a site sample. The white line is the enclosure of the area that failure occurs at least once in all 200 test cases. The larger uncertainty (larger \( \alpha \) ) in the permeability distribution leads to larger uncertainty of shear-slip failure area. In all three cases, the failure zone concentrated near the depths of \(-2240\) m to \(-2340\) m and \(-2440\) m to \(-2490\) m because the permeability is about 2 orders of magnitude lower in these two area than it is in other aquifer locations (Fig. 10).

4. Conclusions

For the analysis of input parameter sensitivity, we used our coupled hydro-mechanical model to simulate 256 cases with
different combinations of the five input parameters. Results of the sensitivity analysis show that the aquifer permeability has the highest score of importance and is the most important factor for injection pressure, displacements, and the potential shear-slip failure for CO₂ sequestration. A smaller permeability value can significantly increase the injection pressure and deformation and leads to a much higher risk of shear-slip failure or fracturing earlier in the life of an injection well. Aquifer thickness is the second most important factor to affect the maximum injection pressure and maximum value of QUOTE , while aquifer porosity is the second most important factor to impact the displacement, and Young’s modulus is ranked third.

To evaluate the impact of a structure of layering aquifer permeability distribution, we studied the effects of aquifer permeability uncertainty (quantified by parameter QUOTE ) on geomechanical deformation and the failure zone through a total of 600 different permeability distributions. Simulation results show that a larger QUOTE leads to larger variation of both the vertical and horizontal displacements, and also leads to a larger uncertainty of shear-slip failure area.

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