GHGT-10
Numerical simulation on the long-term behavior of CO$_2$ injected into a deep saline aquifer composed of alternating layers

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Abstract

In this study, numerical simulations are conducted to predict the long-term behavior of CO$_2$ injected into a deep saline aquifer composed of alternating sandstone and shale layers. We carried out a base-case simulation with a conceptual model broadly based on the geological structure underlying the Tokyo Bay area and sensitivity analyses of key parameters. The results show that alternating layers of moderate permeability and capillary pressure without a structural trapping also has considerable capacity of CO$_2$ storage and seal.

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Keywords: geological storage of CO$_2$; deep saline aquifer; alternating layers; long-term behavior of CO$_2$; numerical prediction

1. Introduction

Alternating relatively thin layers of sandstone and shale/mudstone are considered as another target for CO$_2$ storage in deep saline aquifers in addition to a single combination of thick reservoir and impermeable cap-rock. If the permeability and capillary pressure of the shale layers are moderate, the CO$_2$ plume gradually migrates upward through the layers during the shut-in period. Although CO$_2$ trapping is partial under each shale layer, all of the injected CO$_2$ will be trapped before reaching shallow depths by multi-layers if dissolution and residual gas mechanisms work sufficiently. Because this type of geological storage is expected to have large potential around the world, it is important to evaluate its capacity of CO$_2$ storage and seal.

In this study, we carried out numerical simulations to predict the long-term behavior of CO$_2$ injected into a deep saline aquifer composed of alternating sandstone and shale layers. To perform realistic simulations of the CO$_2$ behavior, we need field information such as geological structure, the hydrological and mechanical properties of the underground formations, the chemical properties of the native fluids, the subsurface distributions of pressure and temperature, the locations of faults, etc. These parameters are known to be site-specific and to take a wide range of values among the potential sites of geological storage. Therefore, we also conducted sensitivity analyses to study the effects of these key parameters on the CO$_2$ behavior.

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2. Model setup

We constructed a simple two-dimensional model representing 2000 meters of alternating sandstone and shale layers based broadly upon the geological structure underlying the Tokyo Bay area in Japan, as shown in Figure 1. The topmost 300-meter region is composed of the unconsolidated sediments, and the thickness of each alternating sandstone and shale layers is 100 meters in the base case, except the topmost sandstone layer of 50 meter. Alternating layers lie flat in the base case.

Relative permeability models of CO$_2$ and water are represented by Corey and van Genuchten type curve (shown by solid line and dash-dotted line in Figure 2 (a)), respectively, as follows;

\[
k_{rg} = \left[1 - S^g\right] \left[1 - S^2\right] \\
S = \frac{S_w - S_{wr}}{1 - S_{wr} - S_{gr}}
\]  

(1),

\[
k_{rw} = \sqrt{S^w \left\{1 - \left[1 - \left(S^w + 1\right)^{1/\lambda}\right]\right\}^2}, \quad S^* = \frac{S_{w} - S_{wr}}{1 - S_{wr}}
\]

(2),

where \(k\), \(S\) and \(S^*\) are the relative permeability, the saturation and residual saturation, respectively. Subscripts “\(g\)” and “\(w\)” indicate water and CO$_2$ respectively. \(\lambda\) is an exponent coefficient and is set to be 0.40. In the base case, residual saturation of CO$_2$ and water are set to be 0.1 and 0.2, respectively. Concerning these parameters, we refer to the papers: [1], [2], etc.

Compressibility of all rocks is set to be $10^{-9}$ Pa$^{-1}$ in the base case. Model of capillary pressure is represented by van Genuchten type curve, as follows;

\[
P_{cap} = -P_0 \left[\left(S^r\right)^{1/\lambda} - 1\right]^{1-\lambda}
\]

(3).

Figure 2 (b) shows the capillary pressure assumed for the shale. In the base case, \(P_0\) is set to be 62 kPa (shown by solid line in Figure 2 (b)). Vertical permeability and capillary pressure of shale is moderate in the base case, assuming that it is composed of sandy shale and shaly sandstone. This shale does not work as a perfect seal by itself.

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Figure 1 Conception diagram of the geological model (parameter values corresponds to the base case).
3. Results and Discussions

3-1 Base case

Figure 3 shows the plume evolution in the base case; snapshots after (a) 50, (b) 500, (c) 950, and (d) 1050 years. In the base case, the permeability of each shale layer is set to be relatively large value (1 md). During several hundred years of shut-in period, CO₂ plume slowly migrates upward due to buoyancy and passes through not only the shale layer just above the injection zone but also the second upper shale layer. However, all of the injected CO₂ is trapped by the dissolution and residual gas mechanisms after 950 years, and does not reach the bottom of the shallowest aquifer (sandstone layer) at the depth of 450 meters. At the bottom of each shale layer, the differences of permeability and capillary pressure serve a barrier for CO₂ plume, resulting in CO₂ accumulation at the top of the underlying sandstone layer. If the geothermal gradient is 20 K/km, the CO₂ plume reaches a depth (about 750 meters) where the pressure and temperature are in the range of liquid-CO₂ condition, resulting in substantial increase in the density and slow down of the upward migration. The accumulation of CO₂ below a shale layer is largely enhanced at this level and brings about larger relative permeabilities of CO₂ due to increased CO₂ saturations. As a result, the CO₂ plume widely spreads horizontally forming a relatively thin layer (the thickness of which is less than a few ten meters). If this occurs, the fraction of CO₂ remained as relatively immobile liquid phase is significantly increased after several hundred years of shut-in as shown in Figure 4 (a). Figure 4 (a) also shows CO₂ dissolution progress during the shut-in period because of more contact with the native groundwater mainly caused by the upward migration.

Figure 4 (b) shows change in pressure from initial state at the top of the reservoir. The extent of pressure buildup region is much larger than that of CO₂ plume itself, which is indicated by the flexion point. The maximum buildup in the base case is about 3.3 MPa (which is substantially smaller than the representative value of fracture pressure). This pressure buildup is relaxed immediately after the shut-in, and re-inflow of water occurs in the region where CO₂ migrates upward through the shale layer and the pressure becomes even smaller than that under the initial state. The pressure is almost restored after 1000 years of shut-in when the migration of CO₂ is almost stopped. Figure 5 shows the...
contour maps of change in pressure from the initial state. It shows that the vertical extent of pressure buildup region is also substantially larger than that of CO$_2$ plume after 50 years (Figure 5 (a)).

![Figure 3 Contour maps of CO$_2$ saturation in the base case after (a) 50 years (when the injection ceased), (b) 500 years, (c) 950 years, and (d) 1050 years in the base case. The liquifed-CO$_2$ region is highlighted by black lines.](image1)

![Figure 4 (a) Time history of mass distribution of each CO$_2$ phase and (b) change in pressure at the top of the reservoir in the base case.](image2)

![Figure 5 Contour maps of pressure change (MPa) in the base case after (a) 50 years and (b) 1050 years in the base case.](image3)

3-2 Sensitivity analyses

Parameters considered in the present sensitivity analysis and their effects on the long-term CO$_2$ behavior are summarized in Table 1. These parameters are particularly influential for an aquifer composed of alternating layers. Here we present some of the results.

The permeability and capillary pressure of the shale layer have large effects on the seal capacity. In the case where vertical permeability of shale is 0.1 md, the upward flow of both water and CO$_2$ is constrained within the injection zone (Figure 6) so that pressure buildup is much higher than that in the base case (Figure 8 (a)). On the other hand, in the case where $P_0$ in the equation (3) of the shale layer is set to be 500 kPa (shown by dash-dotted line in Figure 2 (b))
Table 1 Parameters considered in the sensitivity analysis

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Effect</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Geological conditions</strong></td>
<td></td>
</tr>
<tr>
<td>Geothermal gradient</td>
<td>Large impact on buoyancy &amp; viscosity</td>
</tr>
<tr>
<td>Layer dipping</td>
<td>Flow extension to the updip direction</td>
</tr>
<tr>
<td>Thickness of alternating layer</td>
<td>Large impact on the plume distribution</td>
</tr>
<tr>
<td><strong>Properties of rock</strong></td>
<td></td>
</tr>
<tr>
<td>Porosity of sandstone</td>
<td>Impact on horizontal extension during the injection</td>
</tr>
<tr>
<td>Residual saturation</td>
<td>Impact on mobility and phase distribution</td>
</tr>
<tr>
<td>Relative permeability</td>
<td>Large impact on mobility caused by CO₂ accumulation</td>
</tr>
<tr>
<td>Permeability of sandstone (Horizontal (k_h/) Vertical (k_v))</td>
<td>Small horizontal permeability -&gt; Enhanced vertical flow Vertical -&gt; Impact on accumulation below shale</td>
</tr>
<tr>
<td>Permeability of shale (Horizontal (k_h/) Vertical (k_v))</td>
<td>Vertical -&gt; Large impact on seal capacity &amp; pressure distribution</td>
</tr>
<tr>
<td>Capillary pressure of shale</td>
<td>Large impact on seal capacity in shut-in period</td>
</tr>
<tr>
<td>Compressibility</td>
<td>Larger than water (10⁻⁹ Pa⁻¹) -&gt; Pressure reduction</td>
</tr>
<tr>
<td><strong>Properties of groundwater</strong></td>
<td></td>
</tr>
<tr>
<td>Groundwater composition</td>
<td>Salinity -&gt; Impact on CO₂ dissolution &amp; pressure buildup</td>
</tr>
<tr>
<td>Regional water flow</td>
<td>Small impact at the level of 1cm/yr</td>
</tr>
<tr>
<td><strong>Project design</strong></td>
<td></td>
</tr>
<tr>
<td>Injection (rate/interval)</td>
<td>Injection pressure/Plume footprint</td>
</tr>
<tr>
<td>Injection zone thickness</td>
<td>Injection pressure</td>
</tr>
<tr>
<td>Injection depth</td>
<td>Shallow injection -&gt; Large buoyancy in shut-in period</td>
</tr>
</tbody>
</table>

Figure 6 Contour maps of CO₂ saturation after (a) 50 years and (b) 1050 years in the case that \(k_v = 0.1\) md for shale.
retaining the shale permeability to that of the base case, water can flow out of the reservoir. During the injection period, injection pressure exceeds the capillary pressure and CO₂ extends to upper and underlying shale layers (Figure 7 (a)). However, in the shut-in period, the pressurization due to buoyancy does not exceed the capillary pressure so that CO₂ remains under the second upper shale layer (Figure 7 (b)). Pressure buildup in this case is almost the same as the base case (Figure 8 (b)).

If the layers are inclined (Figure 9 (a)), CO₂ plume widely develops in the updip direction. Figure 10 shows the plume evolution with the layer dipping of 7°. Plume reaches the topmost aquifer, but does not penetrate the unconsolidated sediment with the shale permeability of 1 md (Figure 10 (a)). However, when the vertical permeability of shale layers is 0.1 md, the plume is so constrained within the sandstone layer that it extends largely in the updip direction, reaching the spill point at the ground surface (Figure 10 (b)).

The relative permeability of the sandstone layer and the geothermal gradient also show considerable effects on the CO₂ mobility, consequent distribution of CO₂ plume and amount of CO₂ trapped by the dissolution mechanism. In the case where the straight-line function is assigned to the relative permeability of the sandstone (shown in Figure 2 (a)), lateral evolution below the shale layer is so enhanced that the vertical movement is largely limited (Figure 11 (a)). This straight-line model is an extreme example, however, what model should be adopted to the relative permeability is a big concern. For example, when we give it hysteresis effect (the gas residual saturation differs between the processes of drainage and imbibition), it also has considerable impact on the CO₂ saturation in the pore and CO₂ mobility.

In the cases that CO₂ migrates upward through the layers, the geothermal gradient has a large impact on the behavior. In the case where the geothermal gradient is 30 K/km, the liquefied-region disappears and the upward migration of CO₂ is enhanced by larger buoyancy. Consequently, CO₂ plume reaches the topmost aquifer, although it still does not reach the unconsolidated sediment (Figure 11 (b)).

The thickness of each sandstone and shale layers is another influential factor. If the thickness is comparable to the thickness of the accumulated CO₂ region beneath the shale layer, the volume fraction of the CO₂ region in each sandstone layer (“storage efficiency”) will become much larger. In a case that the thickness of each sandstone and shale layers is assumed to be 10 meters (which is observed in a portion of the Tokyo Bay area) (Figure 9 (b)) instead of 100 meters assumed for the base case, the upward migration during several hundred years of shut-in is largely reduced compared to the base case (Figure 12 (a)). Although the average permeability of the 100-m thick injection zone is lower than the base case, the maximum pressure buildup is almost equivalent to the base case (Figure 12 (b)).

Figure 7 Contour maps of CO₂ saturation after (a) 50 years and (b) 1050 years in the case that \( P_0 = 500 \) kPa for shale.

Figure 8 Pressure buildup at the top of the reservoir in the case that (a) \( k_v = 0.1 \) md and (b) \( P_0 = 500 \) kPa for shale.
Figure 9 Geological model of the case where (a) the layer dipping of 7° and (b) the layer thickness of 10 m is assumed.

Figure 10 Contour maps of CO$_2$ saturation after 1050 years in the dipping case with the shale permeability $k_v = (a)$ 1 md and (b) 0.1 md.

Figure 11 Contour maps of CO$_2$ saturation after 1050 years in the case with (a) relative permeability model of straight-line function and (b) $\text{grad } T = 30 \text{ K/km}$.

Figure 12 (a) Contour map of CO$_2$ saturation after 1050 years and (b) pressure buildup at the top of the reservoir in the case that the thickness of each layer is 10 m.
CO₂ solubility varies depending on the pore fluid salinity, from fresh water to the saturated brine (Figure 13 (a)). If a larger part of the injected CO₂ remains as gaseous state due to high salinity, pressure relaxation after the shut-in will take more time, which is shown in Figure 13 (b).

![Figure 13](image)

Figure 13 Difference of (a) mass of dissolved CO₂ and (b) change in pressure at the top of the reservoir after 100 years depending on the pore fluid salinity (S). In (b) black line for S = 0.032 and blue line for S = 0 are almost overlapped to each other.

We don’t present all of the results of the sensitivity analysis due to a limitation of space. Other parameters, such as the compressibility of rock and those related to the project design, have also considerable impacts. If the compressibility of rock is larger than that of water, the pressure buildup will be reduced. However, its effect on the distribution of CO₂ plume is small. The rate and interval of injection and the thickness of injection zone have also notable effects on the pressure buildup.

4. Conclusion

In this study, we conducted numerical simulations on the long-term behavior of CO₂ injected into a deep saline aquifer composed of the alternating sandstone and shale layers. The results show that this type of aquifer has considerable capacity of CO₂ storage and seal so long as each shale layer has moderate permeability and capillary pressure and the horizontal continuity of each layer is sufficient. Pressure buildup and its propagation are another concern, which show different behavior to the CO₂ plume itself. Sensitivity analyses show that the geothermal gradient and the thickness of each layer have large impacts on the long-term behavior as well as the permeability, capillary pressure, and relative permeability. Solubility of CO₂ depends on the pore fluid salinity, which is influential on the phase partitioning of CO₂ particularly during the post-injection period. Since change in pH caused by CO₂ dissolution is considered to have large effects on the geochemical processes, this will be addressed as a future work.

Reference list: