Abstract

Safely sequestering CO$_2$ in a deep saline aquifer requires calculating how much CO$_2$ the aquifer can store. Since offsetting nationwide emissions requires sequestering large quantities of CO$_2$, this calculation should apply at the large scale of geologic basins. The only method to calculate storage capacity at the basin scale, however, is not derived from multiphase flow dynamics, which play a critical role in CO$_2$ storage. In this study, we explain a new model to calculate basin-scale storage capacity that is derived from flow dynamics and captures the dynamic phenomena of gravity override and capillary trapping. Despite the fact that the model is dynamic, it is simple since it is a closed form expression with few terms. We demonstrate how to apply it on the Fox Hills Sandstone in the Powder River Basin.

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1. Introduction

A promising technology for reducing anthropogenic carbon dioxide emissions is called geological carbon sequestration (GCS) [1,2]. According to the MIT Coal Study, GCS is the critical enabling technology for coal in a carbon-constrained world [3]. In GCS, CO$_2$ is captured at large sources like coal-burning power plants and stored away from the atmosphere in deep geologic reservoirs. In this study, we focus on particularly attractive types of reservoirs called deep saline aquifers since they are widely distributed and have large storage capacities for CO$_2$ [4].

While the collective capacity of deep saline aquifers is large, the safe deployment of CGS to a particular aquifer requires accurately calculating the storage capacity of the aquifer. This capacity is the result of different physical-chemical mechanisms that trap CO$_2$ in different ways. In a mechanism called structural trapping, the upward
migration of buoyant CO$_2$ is suppressed by low-permeability layers [5]. In another mechanism called capillary trapping, CO$_2$ breaks up into small ganglia that are immobilized by capillary forces [6,7]. In solution trapping, CO$_2$ dissolves in the formation brine [8]. Lastly, in mineral trapping dissolved CO$_2$ reacts with reservoir rocks and ions in the brine to precipitate carbonate minerals [9].

While these mechanisms cause CO$_2$ to be trapped for long times, calculating the amount of CO$_2$ that will be trapped is a major challenge. Currently, calculations suffer from major shortcomings of accuracy, complexity, or scale [10]. Numerical simulations can calculate capacity from structural, mineral, and solubility trapping with reasonable accuracy, but these simulations are complex, require detailed geological information about the aquifer, and are limited to local scales. The only option that can be used at regional and basin scales involves the use of numbers called capacity coefficients that account only for structural trapping. Capacity coefficients are multiplicative factors that relate the total pore volume of a reservoir to the pore volume that will be occupied by trapped CO$_2$ [11]. While in practice the pore volume occupied by CO$_2$ is strongly affected by multiphase flow dynamics, these coefficients do not rigorously account for critical dynamic phenomena like gravity instabilities. As a result, current estimates of storage capacity are highly variable and often contradictory [12].

In this study, we demonstrate a new model to calculate storage capacity. This model applies at the basin scale and is both rigorous and simple. It is rigorous because it is derived from multiphase flow dynamics, and it is simple because it is a closed-form, analytical expression with few parameters. In addition to providing a way to calculate capacity, our model provides a visual way of assessing CO$_2$ storage: it shows the total areal extent of the stored CO$_2$, which we call the hydrogeologic footprint. We demonstrate how to apply this model to calculate the storage capacity of the Fox Hills Sandstone in the Powder River Basin.

2. Trapping Model

We provide a full derivation of our mathematical model in another paper [13]. In this paper, we briefly explain the model at the conceptual level and discuss the geologic setting for which it applies. We also review its assumptions and present the relevant equations.

Our model applies to the geologic setting shown in Figure 1. This setting has three important features. The first important feature is scale. The model applies to CO$_2$ sequestration at the basin scale, which typically involves lengths of tens to hundreds of kilometers. The second key feature is the presence of natural groundwater flow. In our model, CO$_2$ is injected into a deep saline aquifer and, after injection, migrates in the direction of groundwater flow. The third key feature is the pattern of injection wells. We model injection from a line-drive array of wells for
which flow does not vary greatly in the direction parallel to the line drive. This allows us to model the flow in one dimension.

The model captures two important multiphase flow phenomena that occur during sequestration. The first phenomenon is gravity override. Gravity override describes how CO₂ migrates to the top of a reservoir both during and after injection, forming a “tongue” that spreads parallel to the low-permeability caprock. The second phenomenon is capillary trapping. Capillary trapping describes how CO₂ becomes disconnected into immobile globules. It occurs after injection when brine flows into pore space at the trailing edge of the migrating CO₂ plume [14].

As with any simple model that captures complex phenomena, our model includes a number of assumptions. We assume that the reservoir is horizontal, homogeneous, and isotropic, and that the injected plume migrates in the direction of groundwater flow. We assume that fluid viscosities and densities are constant. We assume that there is a sharp interface between the CO₂ plume and the brine (sharp-interface approximation), and that spreading effects due to a nonzero gravity number can be neglected [13]. Lastly, we assume that the CO₂ stored by mineral trapping and solution trapping can be ignored. This assumption is valid at small time scales because solution trapping and mineral trapping operate chiefly at larger time scales [15, p.208].

There are two important equations of the model. The equation to calculate the storage capacity is:

\[ C = \left[ \frac{2M \Gamma^2 (1 - S_{wc})}{(1 - M + M \Gamma^2)} \right] \rho_{CO₂} \phi HW L_{total}, \]  
(1)

where \( C \) is the mass of trapped CO₂, \( \Gamma \) is the trapping coefficient, \( M \) is the mobility ratio, \( \rho_{CO₂} \) is the density of CO₂, \( \phi \) is the porosity, \( W \) is the length of the injection array, \( H \) is the net sandstone thickness of the reservoir, and \( L_{total} \) is the total extent of the CO₂ plume (Fig.1b). We define the mobility ratio as:

\[ M = \frac{1/\mu_w}{k_{rg}/\mu_g} \]  
(2)

where \( \mu_w \) is the viscosity of brine, \( \mu_g \) is the viscosity of CO₂, and \( k_{rg} \) is the endpoint relative permeability to CO₂.

We define the trapping coefficient as:

\[ \Gamma = \frac{S_{rg}}{1 - S_{wc}} \]  
(3)

where \( S_{rg} \) is the residual saturation of CO₂ and \( S_{wc} \) is the connate water saturation.

The term in brackets in Equation 1 is a key feature of our model. It relates total pore volume of an aquifer to the volume of trapped CO₂. We call it the efficiency factor, and it plays a similar role to currently used capacity coefficients.

The second important equation in our model is used to draw the CO₂ footprint. It calculates the distance the plume has migrated away from the well array when it is completely trapped (Fig.1):

\[ L_{max} = \frac{(2 - \Gamma)(1 - M (1 - \Gamma))}{(2 - \Gamma)(1 - M (1 - \Gamma)) + \Gamma^2} L_{total} \]  
(4)

The distance the plume travels during injection \( L_{inj} \) is then given by:

\[ L_{inj} = L_{total} - L_{max} \]  
(5)
3. Storage Capacity of the Fox Hills Sandstone

3.1. Geohydrologic Setting

The Fox Hills Sandstone occurs in the Northern Great Plains. In this study, we calculate storage capacity for deep parts of the formation in the Powder River Basin. This basin is an asymmetric foreland basin that lies in Montana and Wyoming.

The Fox Hills Sandstone is Upper Cretaceous in age. Its composition differs in detail in different areas, but in general it consists of massive, fine- to medium-grained sandstone with siltstone and minor shale, which are sometimes interbedded [16, p.T68]. The depth to the top of these rocks, and the net sandstone thickness, is shown in Figure 2.

The formation is conformably overlain by and intertongued with the Hell Creek Formation in Montana and the Lance Formation in Wyoming [16, p.T68]. These formations differ only in geography and provide an extensive top seal called the Upper Hell Creek Confining Layer [18, p.82]. The Fox Hills is conformably underlain by marine shale and siltstone in the Lewis Shale or Pierre Shale, which form an aquiclude [19, Plate II].

Porosity in the Fox Hills Sandstone is poorly known. We found data for only the West Side Canal Field in the Green River Basin, in which the porosity is reported to be 0.21 [20, qtd. in 17]. The flow direction over most of the basin is south to north, as shown in Figure 3. In the southern part of the basin, however, the flow direction is from west to east.

3.2. Capacity Calculation

The first step in calculating the storage capacity of the Fox Hills Sandstone is identifying the spatial domain over which to apply the model. We do this by drawing boundaries around the aquifer based on three criteria: the likelihood of CO2 leakage, the uniformity of the regional flow direction, and the depth of the formation. These boundaries are shown in Figure 4. To limit leakage, we draw boundaries at outcrops [21, Fig.10], large faults [21, Fig.10], and places where the caprock contains more than 50% sand [17, Map c8foxhillsg]. While the leakage properties of faults and sandy parts of the caprock are unknown—faults, for example, may in general be conduits or barriers for flow—we identify these features as boundaries to be safe since little or no data is available to evaluate the leakage risk.

In addition to drawing boundaries based on leakage, we draw boundaries where the regional flow direction is non-uniform since our model assumes a uniform flow direction. Based on this criterion, we draw a boundary in the

![Figure 2](image-url). Depth and net sandstone thickness in the Fox Hills Sandstone. (a) Modified from [17, Map c1foxhills]. (b) Modified from [17, Map c4foxhillsg].
southem part of the basin where the flow direction abruptly changes, and a boundary at the northern part of the basin where the streamlines sharply converge (Fig. 3).

We draw the last type of boundary where the top of the reservoir is 800m deep. Assuming a hydrostatic pressure gradient and a geothermal gradient of 25°C/km, this is the depth at which CO2 becomes a supercritical fluid. We define it as a boundary to ensure that CO2 is stored efficiently in a high-density state.

All of the boundaries constrain both the placement of injection well array and the migration of the CO2 plume except for the depth boundary. We choose this boundary to constrain only the placement of the well array. This is because using it to constrain plume migration would unnecessarily limit the portion of the reservoir used for storage: since most of the injected CO2 is stored in the vicinity of the well array [13], allowing the thin leading front of the plume to migrate above 800m depth will not strongly affect the storage efficiency of most of the plume.

After identifying the boundaries of Fox Hills Sandstone, we set values of the input parameters in the trapping equation (Eq. 1). Our methodology involves two key features. The first key feature is the source of the data we use to set the parameters. We set some of the parameters based on data from the formation itself, and set others based on laboratory experiments since the relevant data does not exist for the formation. The second key feature is how we handle variability and uncertainty. Since geologic data can be highly uncertain and the parameters in the model can vary widely at the basin scale, handling variability and uncertainty is a major challenge for our model. For parameters set based on experiments, we address this challenge by using a range of values that covers the range of experimental findings. For parameters set from reservoir data, we use average values for the formation taken from the area within the 800m-depth boundary, where most of the CO2 will be stored.

We set the following parameters based on laboratory data: the connate water saturation $S_{wc}$, the residual CO2 saturation $S_{rg}$, and the endpoint relative permeability to CO2 $k_{frg}$. The data we use are from Bennion and Bachu [22]. We use this data to posit three scenarios consistent with minimal CO2 trapping, maximum trapping, and average trapping. These scenarios and the values we use for the parameters are listed in Table 1, along with the resulting trapping coefficients (Eq. 3). We use each of these scenarios to calculate a minimum, maximum, and average storage capacity.

We set the remaining parameters based on data from the reservoir (Table 2). We set porosity to 0.21, assuming that the only measurement we found is representative of the formation in the absence of other data. We set the net sandstone thickness to 120m based on the map in Figure 2. Lastly, we calculate the density of CO2 and the mobility ratio as functions of temperature and pressure in the reservoir. We calculate temperature in the reservoir to be about 66°C using a geothermal gradient of 35°C and an average formation depth of 1500m [23]. We calculate pressure to be 15 MPa using a hydrostatic gradient. With this temperature and pressure, we calculate the density of CO2 using an online thermophysical property calculator provided by MIT [24]. We also use the calculator for the viscosity of CO2, and use a correlation function to calculate the viscosity of brine [25]. We then use these viscosities, together with the endpoint relative permeability to CO2 from our average-trapping scenario (Table 1), to...
Table 1. Trapping scenarios and the corresponding CO2-brine displacement parameters.

<table>
<thead>
<tr>
<th>Trapping Scenario</th>
<th>$S_{wc}$</th>
<th>$k_{rg}$</th>
<th>$S_{rg}$</th>
<th>$\Gamma$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Less Trapping</td>
<td>0.5</td>
<td>0.5</td>
<td>0.2</td>
<td>0.40</td>
</tr>
<tr>
<td>Average Trapping</td>
<td>0.3</td>
<td>0.7</td>
<td>0.4</td>
<td>0.57</td>
</tr>
<tr>
<td>More Trapping</td>
<td>0.4</td>
<td>0.6</td>
<td>0.3</td>
<td>0.50</td>
</tr>
</tbody>
</table>

calculate the mobility ratio (Eq.2).

The final parameters to set in our equation are the width of the injection well array $W$ and the total extent of the CO2 plume $L_{\text{total}}$ (Fig.1). The width of the injection well array is constrained by the smallest distance between the boundaries perpendicular to the flow direction. This constraint restricts CO2 from crossing a boundary during migration of the plume. We measure it to be about 42 km. The total extent of the plume $L_{\text{total}}$ is constrained by the distance between boundaries parallel to the flow direction. We measure it to be about 299 km.

We now have all of the parameters required to calculate storage capacity using Equation 1. For the average-trapping scenario, we calculate the storage capacity to be about 5 gigatons of CO2 and the efficiency factor to be about 1.2%. Table 3 lists the results for the other trapping scenarios.

3.3. Hydrogeologic Footprint

To draw the hydrogeologic footprint, we first calculate the extent of the trapped plume $L_{\text{max}}$ using Equation 4. For the average trapping scenario, we calculate $L_{\text{max}}$ to be about 253 km. As shown in Figure 5, we draw the footprint of the trapped plume by measuring out this distance from the well array along streamlines, since the CO2 will migrate with the regional ground water flow. We next calculate the extent of the injection plume $L_{\text{inj}}$ using Equation 5. For the average trapping scenario, we calculate $L_{\text{inj}}$ to be about 46 km. We draw the footprint for this plume by measuring out the distance $L_{\text{inj}}$ on both sides of the well array (Fig.5). We measure this distance perpendicular to the array because the pressure gradient from injection drives flow during the injection phase, and this gradient will predominantly point perpendicular to the array.

4. Discussion

Our model for calculating storage capacity has both advantages and disadvantages. One disadvantage is that its assumptions are fairly restrictive. For example, it assumes that solubility and mineral trapping are unimportant at small timescales. Also, it assumes the aquifer is horizontal, which means it neglects migration of CO2 upslope due to any non-zero dip in the caprock. Another disadvantage is that the uncertainty in the capacity estimates is fairly large. As shown for the Fox Hills Sandstone, the difference between the upper and lower capacity estimates is about 3 gigatons of CO2 (Table 3).

While the model has shortcomings, it has significant advantages over using capacity coefficients, which is the only other technique currently available for calculating capacity at the basin scale. One advantage is that it is simple to apply since it is a closed form expression with few terms. Using capacity coefficients, however, is difficult since

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\phi$</td>
<td>0.21</td>
</tr>
<tr>
<td>$H$</td>
<td>120 m</td>
</tr>
<tr>
<td>$W$</td>
<td>42 km</td>
</tr>
<tr>
<td>$L_{\text{total}}$</td>
<td>299.3 km</td>
</tr>
<tr>
<td>Average-trapping $M$</td>
<td>0.26</td>
</tr>
<tr>
<td>$\rho_{\text{CO}_2}$</td>
<td>540.5 kg/m$^3$</td>
</tr>
</tbody>
</table>
there are almost no published values of coefficients in the literature and there is no rigorous way of deriving them [10]. The only published values we found come from the Carbon Sequestration Atlas by the National Energy Technology Laboratory (NETL), but the derivation of these values is unclear [11]. Another advantage is that our model produces physically meaningful estimates since it is based on multiphase flow dynamics. Capacity coefficients, on the other hand, either ignore dynamics or use overly simple multiplicative factors to account for dynamics. For example, the NETL multiplies the total pore volume of an aquifer by factors between 0.6 and 0.4 to account for gravity instabilities [11]. The final advantage of our model is that it is based on reservoir-specific geohydrology. While capacity coefficients should also be reservoir-specific, in practice the NETL uses the same capacity coefficients for all reservoirs [11].

<table>
<thead>
<tr>
<th>Scenario</th>
<th>Efficiency Factor (%)</th>
<th>Capacity (gigatons)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Less Trapping</td>
<td>0.8</td>
<td>3.3</td>
</tr>
<tr>
<td>Average Trapping</td>
<td>1.2</td>
<td>5.0</td>
</tr>
<tr>
<td>More Trapping</td>
<td>1.6</td>
<td>6.4</td>
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Works cited