Utilizing Multiphase Flow Modeling to Estimate CO₂ Solution Storage Efficiency and Sequestration Project Size

Introduction

Carbon Capture and Storage (CCS) has been in the spotlight recently. The United States aims to reduce greenhouse gas (GHG) emissions as a climate change mitigation strategy. There are powerful federal and state incentives to develop CCS projects. Through the Inflation Reduction Act (IRA) of 2022, facilities that capture and sequester CO₂ can qualify for federal tax credits(45Q). State incentives are also under programs such as the Low-Carbon Fuel Standard (LCFS) and Sustainable Aviation Fuel (SAF). CCS prevents CO₂ emissions from entering the atmosphere, promotes CCS owners/operators as environmental stewards, and helps foster economic growth. CO₂ producers and emitters should consider how to maximize the benefits of CCS and how it will ultimately help your company meet its sustainability goals with the support of environmental engineers and consultants.

Geologic sequestration (GS) is the injection of captured CO₂ in the supercritical phase into deep geologic units for permanent storage via a Class VI injection well. The permitting effort for a Class VI well requires computational modeling to delineate the area of review (AOR), informed by the maximum extent of the injected CO₂ plume and areas where the pressure in the reservoir can be elevated enough to push fluids up through flaws or penetrations of the caprock and potentially endanger underground sources of drinking water (USDWs).

As the supercritical CO_2 is a separate buoyant phase from the media within the storage unit, a model capable of computing multiphase flow is required to assess how this buoyant CO_2 will behave and migrate in the subsurface. Since we can assess CO_2 migration and the ultimate fate of injected CO_2 via this modeling, it will also be a valuable application for project sizing.

CCS projects involve detailed planning, big money, and a high degree of risk, particularly in the earlier stages of a project. Assessing the mechanisms leading to the most safe and efficient sequestration of captured CO_2 is a vital component of a carbon capture and storage (CCS) project. Fortunately, understanding CO_2 storage efficiency and capacity estimates will help you properly scope your project location and maximize the benefits of CCS.

Deep CO₂ Trapping and Storage

To estimate long-term storage capacity, we must consider the various CO₂ trapping mechanisms:

Trapping Mechanism	Mechanism Description	
Structural/Stratigraphic	Faults, Folds, Unconformities, Pinch-Outs	
Residual (Capillary)	CO ₂ immobilized in reservoir pore space	
Solution (Solubility)	Supercritical CO ₂ phase dissolves into the reservoir's native aqueous phase	
Mineral	CO ₂ reacts with reservoir media to form new solid phases	

Table 1.CO2 Trapping Mechanisms

The mechanisms in Table 1 are generally ordered from least to most storage security (see Figure 1 below). As such, mineral trapping provides the highest degree of storage security; however, it is a mechanism that may not significantly come into play until long after injection ends and is dependent on the geochemistry of the reservoir. Under most conditions, solubility trapping is the ultimate long-

term trapping mechanism for injected CO_2 due to the dissolution of the separate supercritical phase. Estimating solution storage efficiency will be a key metric for CCS project scoping.

Here, we look at using multiphase flow modeling to estimate design and operational parameters that will lead to the most efficient use of pore space. We calculated solution storage efficiency as a percentage by determining how many model cells reach full CO₂ saturation at the end of model time. With the solution storage efficiency estimate and what we know about total available pore space through the geology, we also estimated the total solution storage capacity of the CCS project site in the case study presented herein.

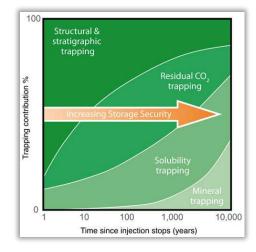


Figure 1 - From Intergovernmental Panel on Climate Change (IPCC) Report on CCS (2005).

Case Study - Investigating Efficient Use of Reservoir Pore Space

For this CCS project example, we developed a simple geologic model of the site that includes the reservoir and the upper confining zone (Figure 2 below). We built the model using the TOUGH2 simulator (Lawrence Berkeley National Laboratory) within the PetraSim graphical interface (RockWare®). In this model, we built the geologic layers (reservoir and confining zone), assigned appropriate material properties, and calculated initial conditions. For this case study, we investigated what factors may promote solution storage efficiency under these particular geologic conditions across six hypothetical Class VI injection wells. Specifically, we looked at whether injection rate, duration, and location make a difference, and whether injecting into multiple wells rather than a single well makes a difference.

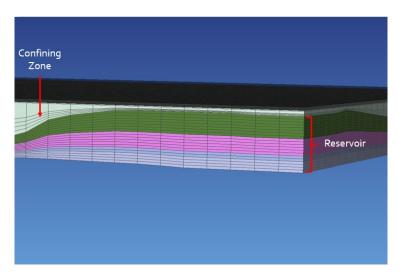


Figure 2 - Capture of a simple geologic model from PetraSim.

Injection Rate and Duration

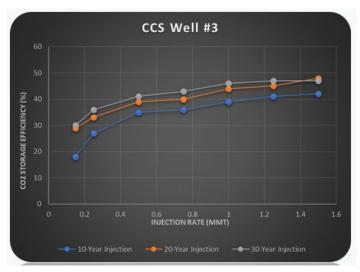
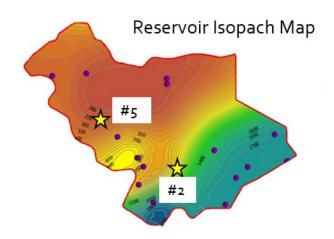


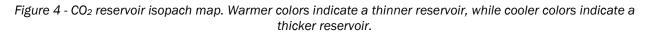
Figure 3 - Graph of example hypothetical well efficiencies across various injection rates and durations.

First, we assessed the injection rate and duration. We modeled various typical injection rates (in millions of metric tons per year, MMT/yr), as shown on the X axis of the graph (Figure 3, left), at hypothetical injection wells over 10, 20, and 30-year injection durations. We then calculated the CO₂ solution storage efficiency as a percentage, as shown on the Y-axis. We found that at each well, the injection rate and duration make a difference. In these cases, the 20-year injection interval is more efficient than a 10-year interval. However, we do not see an equivalent gain in efficiency by using a 30-year interval in a single well. For injection rates, there is a direct relationship between injection rate and storage efficiency. However, you can see this increase in efficiency with

increasing rate becomes less pronounced quickly, and generally, in this case, rates greater than 1 million metric tons per year (MMT/yr) do not increase efficiency in a single well.



Injection Location



Next, we assessed whether or not injection location makes a difference in efficiency. This case looks at a scenario of a thicker reservoir on the east side of the project location and a thinner reservoir on the west side (Figure 4 above). We modeled three wells on each side, with two examples in Figures 4 (above) and 5 (below). When using the same operational parameters in these locations, the thinner reservoir areas consistently show more efficient solution storage by about 10%. But, we are seeing higher efficiency because the CO₂ plume can migrate upwards to the caprock and spread out more quickly, leading to increased dissolution. The caveat is that this also leads to a larger Area of Review (AOR). While efficiency is generally lower in areas with the thicker reservoir, there is more reservoir pore space available and, ultimately, more control over the size of the AOR.

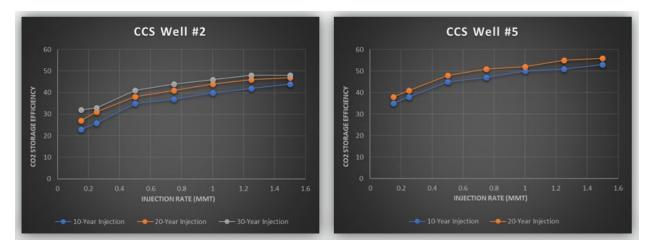


Figure 5 - Graphs of example hypothetical well efficiencies across various injection rates and durations.

Injection in Multiple Wells

Finally, we assessed whether injecting into multiple wells rather than a single well would make a difference in efficiency. We looked at a simpler case of injecting at 1 MMT/yr into the six wells for 20 years. This results in notably higher efficiency than injecting into single wells because we are utilizing more of the available pore space in different locations within the project area. However, there are caveats and considerations for this. The CO_2 plumes begin interacting with each other within five years of initiating injection, and there is a resulting large composite plume that extends well beyond the project boundaries. As you would expect, the pressure front was also notably elevated in this scenario. To make the most efficient use of pore space with multiple wells, we must consider optimizing the individual wells based on variability in site geology and how injecting multiple wells will affect the pressure front and overall CO_2 plume extent.

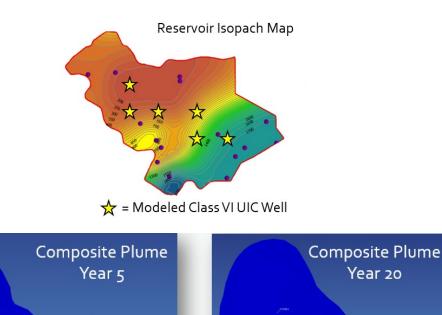


Figure 6 - Composite CO₂ plume across the six hypothetical injection wells.

Project Size Estimation

After completing the efficiency portion of the case study, we also estimated the maximum project size, or sequestration capacity, for this project area (Figure 7 below). We designed this estimation to be at an order of magnitude level to optimize injection well placement, rates, and duration. This calculation considers the desired project area, the porosity of the reservoir, and the total amount of CO_2 that could dissolve in the native reservoir fluids (brine). The metric tons of CO_2 in saturated brine in the project area is the total estimated amount of CO_2 we could inject into the reservoir. However, we made a couple more basic assumptions to reach a more realistic estimate. First, we added an edge effect reduction to provide a buffer, accounting for the fact that the AOR cannot extend past the project boundary. We assumed this to be 75%. Finally, we factored in the solution storage efficiencies we calculated; 45% was used, as this was the approximate average efficiency observed in the case study. The result is a total estimated sequestration capacity of 42 million metric tons.

Project Area	27,509,605	m²
Average Thickness of Reservoir	300	m
Volume of Reservoir (calc)	8,252,881,500	m ³
Volume of Pore Space (calc)	2,475,864,450	m ³
Density of Brine (based on USEPA guidance)	1,040	kg/m³
Weight of Brine in Pore Space (calc)	2.5749E+12	kg
Metric Tons of Brine (calc)	2,574,899,028	metric tons
Wt. % of CO ₂ in Saturated Brine	4.8	weight %
Metric Tons of CO ₂ in Saturated Brine in Project Area	123,595,153	metric tons
Edge Effect Reduction (assumption, 75%)	92,696,365	metric tons
Utilization Reduction (assumption, 45%)	41,713,364	metric tons
Total Estimated Sequestration Capacity	42	million metric tons

Figure 7 - Calculation estimating total sequestration capacity based on storage efficiency.

Case Study Conclusions

In this case study, we found that injection rate, duration, and location make a difference in solution storage efficiency. In this particular case, injecting at 1 MMT/yr for 20 years is ideal for a single well. Figure 8 (below) shows this scenario, with the red areas representing where the CO_2 has dissolved within the formation fluids and showing some additional up-dip migration. Injecting into multiple wells and utilizing more of the estimated sequestration capacity can lead to increased efficiency, but it brings forth considerations for the size of the AOR. Finally, we calculated the total estimated storage capacity based on typical efficiency results observed in the case study.

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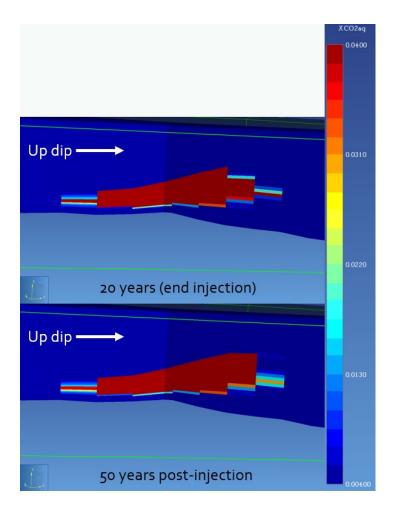


Figure 8 - Transect in PetraSim showing the up-dip plume migration and dissolution of CO₂.

Recommendations

How can you apply the findings from this case study to future CCS projects? When scoping CCS projects and ultimately putting together the permit application, you can utilize the required computational modeling as leverage to help maximize CCS's economic and environmental benefits. To do this effectively, you will need to develop an understanding of your site geology. Then, build the basic model to investigate injection rates, durations, and locations that will maximize CO₂ solution storage efficiency to meet the needs of your specific project. Finally, you can use this to estimate your site's total sequestration capacity to give you an idea of the overall potential project size.

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