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Impact Analysis of Simulation Parameters on Supercritical Carbon Dioxide Storage Modeling in Aquifers

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Abstract

This study presents an in-depth analysis of the variability in numerical simulations of supercritical carbon dioxide injection and storage. The project focuses on the impact of the grid size and different calculation methods on the outcomes of the simulation. navigator software has been utilized as the simulator of choice, whereas the three simulation models in question were based on the CO2STORE, CO2SOL, and GASSOL (with Henry solubility enabled) keywords. The simulation runs were conducted on a homogeneous, rectangular prism that represented an aquifer. The model underwent a three-year injection process followed by a 100-year-shut-in period that allowed for observations regarding CO_2 plume development and migration. The initial conditions were aligned with the Illinois Basin - Decatur Project. The study compares the efficiency of carbon dioxide dissolution mechanisms across all models as well as highlights the impact of the grid size on the plume area estimations and computational demand.

Keywords: Numerical Simulation, Supercritical CO_2 Injection, Computational Fluid Dynamics, Geological Carbon Storage, Reservoir Modeling

1. Introduction

Carbon dioxide is Earth's second most abundant greenhouse gas after water vapor [1]. It is the second most influential factor in contributing to the phenomenon of global warming as well as climate change [1]. According to the report issued by the Intergovernmental Panel on Climate Change (IPCC), there has been a significant increase in CO_2 emissions from human activities - 35% in 30 years since 1990 [2]. Such a steep rise is accounted to be one of the main reasons for the observed increase in total atmospheric carbon dioxide volume. The authors of the statistics claim that the emissions from the combustion of fossil fuels for energy and transportation are the two main sources of human-created pollution. Moreover, the authors also emphasize that such a rise in CO_2 emissions has a widespread impact on modern society through rising temperatures, sea level rise, more frequent extreme weather events, or biodiversity loss [2]. Therefore, understanding the causes, consequences, and solutions of carbon dioxide (as well as other greenhouse gases) from human activities is crucial, just as acting to reduce and adapt to the already-existing changes. There are several methods to combat challenges of this nature, and the CCUS projects have gained a lot of interest and funding in the last two decades [3]. The abbreviation stands for Carbon Capture, Utilization, and Storage, and it describes a group of projects targeting placing carbon dioxide in places where its impact on global warming is negligible. It has become recognized as an important solution to constantly rising atmospheric carbon dioxide emissions. CCUS projects can provide cuts in emissions that could potentially allow for stabilization of greenhouse-gas levels to make the continued use of fossil fuels permissible [4]. Operations like these are carried out in several steps. Firstly, the carbon dioxide must be captured, usually at a power plant or another industrial facility. Then, it is transported to a storage site, typically through a pipeline [5]. Throughout the years, CO_2 storage has been implemented in different forms, such as terrestrial, oceanic, and geological sequestration attempts. However, in this project, the geological storage of carbon dioxide will be the focal point of the discussion.

Unfortunately, the term geological is not specific enough because the CO_2 in question can be stored in depleted oil reservoirs, coal seam beds, and saline aquifers. Each type of storage location has a dichotomy of benefits and drawbacks [6]. For instance, depleted

oil and gas reservoirs are deemed the safest since they have been able to accumulate and cap hydrocarbons for an extended period. Additionally, already existing computer models are a tremendous help with history matching and greatly improve the accuracy of storage estimates [3]. On the other hand, they offer limited storage capacity. The unmineable coal beds are suffering from the same problem to an even greater extent, which is only worsened by the risk of CO_2 leakage due to coal swelling and fracturing. Among all storage solutions, saline aquifers are characterized by the highest sequestration capabilities [5,7]. Their global storage capacity is far superior to the other two types of reservoirs mentioned and has been estimated to be between 4,000 and 23,000 Gt [8]. Salinity in such reservoirs does not facilitate the carbon dioxide solubility capabilities in water however, the aquifers in question must be saline to be eligible for sequestration rather than industrial, agricultural, or human purposes [9-11] Therefore, this project focuses on the injection of CO_2 into saline aquifers for the purpose of geological carbon storage. Carbon dioxide can be injected into a reservoir in all phases. The gaseous and solid phases are not economically feasible and are not considered in the context of carbon storage. The injection of CO_2 in a liquid phase is not widely used in the carbon storage industry, but it has been proposed as a possible alternative to other methods, promising simplifications along the supply chain [12]. Another more experimental solution is to inject pre-dissolved carbon dioxide into the aquifer. On paper, it offers many advantages, such as increasing the stability within the reservoir by decreasing the buoyancy of carbon dioxide and effectively reducing the risk of upward migration of the plume. Moreover, injecting dissolved carbon dioxide into brine is also expected [13]. It can also provide improved safety for such operations as it reduces the mobility of carbon dioxide, preventing it from escaping through a fracture network. However, this approach presents a plethora of challenges and drawbacks, with pressure build-ups and increased costs, to name a few [14]. Therefore, in this project, the injection of supercritical carbon dioxide is taken into consideration. In this case scenario, the CO_2 is raised to a temperature above 87.76 °F and a pressure of 1,070.0 psi [15]. In that state, it can expand to fill its container like a gas would while maintaining density like a liquid. Because of these properties, it can fill the pores of rock strata more efficiently than a liquid phase with a reduced risk of upward migration due to the higher mass per volume occupied. On top of that, supercritical carbon dioxide can be characterized by high solubility and diffusivity, and it easily penetrates pore spaces of the rock due to its low viscosity [16]. All of which are greatly desired characteristics in storage applications [17]. These qualities make supercritical carbon dioxide a great candidate for storage applications.

This project focuses on numerically simulating geological carbon storage by injecting supercritical CO_2 into a deep saline aquifer. In principle, there are multiple ways to tackle a problem like this through commercial and open-source software that can model geological carbon storage. For instance, GEM from Computer Modeling Group, VIP-Comp created by Halliburton, TOUGH2 codes from Lawrence Berkeley National Laboratory, and Eclipse developed by Schlumberger can all help achieve goals such as modeling the GCS. However, this project utilized tNavigator software created by Rock Flow Dynamics. It enables parallel processing functionality that allows the running of complex and large projects relatively fast and offers backward compatibility for Eclipse code, which is helpful when it comes to history matching with projects done in the past. The simulation engine created by Rock Flow Dynamics offers enhanced functionality of the package created by Schlumberger. Therefore, the structure of the code and keywords remain mostly unchanged, which allows for a less steep learning curve for a new user.

In this paper, with the help of navigator software, the injection of supercritical CO_2 into a water reservoir was simulated using three different methods - CO2STORE, CO2SOL, and GASSOL (with Henry solubility enabled) keywords. Then, the results were compared, and a sensitivity analysis with respect to the grid size was performed to determine how these models differ. As for early 2024, academic publications on carbon storage simulations performed in this software have not been found. Moreover, scholarly articles comparing storage methods against one another on the same grid are also very scarce. This study aims to Therefore, this project can help cast light on varying calculation methods to determine the appropriate one for the task at hand.

2. Simulation Methodology

2.1 Model Setup

In this study, carbon dioxide was injected into a three-dimensional and homogeneous rectangular prism to minimize the grid and dispersion effects. The injector well, with perforations across the entire reservoir depth, was placed directly in the middle of the grid. In all three cases, the injection consisted of pure carbon dioxide in a supercritical state throughout the three-year injection period, followed by 100 years of shut-in. Each model was initially created with 100% fresh water thoroughly filling the reservoir pores. With that setup, each model's parameters were matched so that each, after three years of carbon dioxide injection at a constant rate, contained the same number of CO_2 moles within the matrix. The PVT data for the simulations was acquired from the Illinois Basin-Decatur Project (IBDP). It is a large-scale geological carbon storage project that is taking place in Decatur, Illinois [18]. In that case, an injection through a singular well into a sandstone formation was modeled using the ECLIPSE simulation package. The data obtained and used in this project comes from the CO_2 Data Share project, which has been gathering information from near-surface monitoring and sampling installations [19]. The relative permeability relationships used in the IBDP project were converted to Corey power-law curves to accelerate the simulation speeds over the hundred years of shut-in period. The parameters required for the equations were obtained by history matching the data from the Illinois Basin. The pore space distribution parameter was equal to 2 since the aquifer has homogeneous properties [20-21]. The initial conditions for all models in this study were 5000 ft, 3000 psia, and 112 °F at the top of the reservoir depth and initial temperature and pressure at that depth, respectively.

The only boundary condition on the model was the maximum pressure within the aquifer that could not exceed 8,700 psia due to a technical constraint on the CO2STORE keyword in one of the models. Table 1, located below, summarizes the initial setup of all models analyzed in this study.

Parameter	Value	Unit
Grid Size	1275 x 1275 x 400	ft
Total Volume	6.50E+08	ft^3
Porosity	25	%
Pore Volume	1.63E+08	ft^3
Permeability X/Y/Z	2000/2000/1000	mD
Rock Compressibility	3.20E-06	psi^{-1}
Initial Temperature	112	°F
Initial Pressure	3,000	psia

Table 1: Initial Parameters of all Models in the Study.

The objective of the study is to compare the different simulation models within the ECLIPSE/tNavigator software package to help determine which is best for different types of applications within the reservoir engineering project. Moreover, this project aims to investigate the effects of grid size variation on each of the numerical methods.

2.2 CO2STORE Keyword

The model that was used in the Illinois Basin - Decatur Project utilized the CO2STORE option within the ECLIPSE simulation software to recreate the actual carbon dioxide injection into the reservoir performed on-site. Hence, it became a starting point for this project as the data used in this calculation method was pulled directly from the real world, helping to validate the further work performed in this study [19]. This simulation method is based on extended solubility correlations performed by Spycher. Their methodology allowed for the derivation of the fundamental equations governing the CO2STORE keyword, y_{H_2O} regarding the molar fraction of water in the gas phase and x_{CO_2} quantifying the molar fraction of carbon dioxide in the water phase, which are:

$$y_{H_2O} = \frac{K^0_{H_2O}}{\phi_{H_2O}P} exp\left(\frac{(P - P^0)\overline{V}_{H_2O}}{RT}\right)$$

$$x_{C_2O} = \frac{\phi_{C_2O}(1 - y_{H_2O})P}{55.508K^0_{CO_2}\gamma'} exp\left(\frac{(P - P^0)\overline{V}_{CO_2}}{RT}\right)$$

In this case, K^0 stands for the equilibrium constant of the component at a given temperature and a reference pressure. $\underline{V}$ describes partial molar volumes of each condensed phase, ϕ is for the fugacity constants of the components, whereas γ' stands for a coefficient that accounts for carbon dioxide activity based on the salinity of the brine [9]. The salts in question are sodium chloride, calcium chloride, and calcium carbonate. Ezrokhi's method is utilized to account for the simultaneous presence of carbon dioxide and salts during the water density and viscosity calculations [22]. The viscosity is calculated in accordance with Lohrenz–Bray–Clark correlation. The CO2STORE keyword allows for 13 total components to be present in a system, which are H_2O and CO_2 as the main hydrocarbon components that can be in both phases (water and gas). Eight ions, which are

Na^+, Cl^-, H^+, HCO_3^-, OH^-, CO_3^{2-}, Ca_2^+, *and* $CaCl^+$, and can only be present in the water phase. Lastly, three solids can be present, $NaCl(s)$, $CaCl_2(s)$, *and* $CaCO_3(s)$ [23]. This model allows these components to participate in the following equilibrium reactions:

$$CO_2 + H_2O \leftrightarrow H^+ + HCO_3^- ,$$

$$HCO_3^- \leftrightarrow H^+ + CO_3^{2-},$$

$$H_2O \leftrightarrow H^+ + OH^-,$$

$$CaCl^+ \leftrightarrow Ca^{2+} + Cl^-.$$

Moreover, the CO2STORE keyword allows for three precipitation/dissolution reactions:

$$NaCl(s) \leftrightarrow Na^{+} + Cl^{-},$$

$$CaCl_2(s) \leftrightarrow CaCl^{+} + Cl^{-},$$

$$CaCO_3(s) \leftrightarrow Ca^{2+} + CO_3^{2-}.$$

These functionalities allow this keyword to represent carbon storage versatilely, covering various phenomena occurring within the aquifer like dissolution, water vaporization, and precipitation of solids. Its most significant advantage is being created explicitly with carbon storage functionality compared to the other models covered in this study. Therefore, this makes this method a good candidate for applications like the Illinois Basin - Decatur Project, or this study.

2.3 CO2SOL Keyword

Whereas the CO2STORE option within ECLIPSE/tNavigator was explicitly built for the purpose of twophase systems (gas and water), the CO2SOL keyword enables carbon dioxide to be soluble not only in water but also in oil if it is defined. In the case of this study, the oil phase was not introduced to maintain continuity and cohesion between the models. The CO2SOL option allows the user to define a solubility table through the SOLUBILI keyword; however, this project opted for a default table that later was adjusted through the comparison of the number of moles injected to correlate with other models. This keyword utilizes the following correlation, developed by, as the backbone of the carbon storage process:

$$R_{sw} = \begin{cases} a \cdot p \cdot \left[1 - b \cdot \sin\left(\frac{\pi}{2} \cdot \frac{c \cdot p}{c \cdot p + 1}\right)\right], \text{if } p < p^0 \\ R_{sw}^0 + m \cdot (p - p_0), \text{if } p \geq p^0 \end{cases}$$

Where *a, b, c*, and p^0 are calculated coefficients and *p* is the actual pressure in psia. Moreover, the work of Chang et al. from 1998 allows for modifications to the density calculations through the utilization of the Ezrokhi's method and the formula derived by Garcia [24].

$$\frac{1}{\rho_{aq}} = \frac{1 - X_2}{\rho_b} + \frac{X_2}{\rho_{CO_2}}$$

X_2 is defined as the mass fraction of the aqueous carbon dioxide, ρ_b and ρ_{CO2} as the densities of brine and dissolved CO_2 respectively. The latter is calculated through a dependance of temperature on the correlation describing the molar volume of aqueous carbon dioxide (Garcia, 2001).

$V_\varphi = a + bT + cT^2 + dT^3$

Here, V_φ translates to the molar volume of carbon dioxide. The T refers to temperature, whereas the *a, b, c, d* are constant coefficients that can be seen in Table 2.

a	b	c	d
37.51	-0.09585	0.000874	-0.0000005044

Table 2: The Constant Coefficient table from Garcia's Method, Utilized for Determining the Density of water Containing Dissolved Carbon dioxide.

Once the molar volume of CO_2 is known, one can calculate the partial density of carbon dioxide through the equation:

$$\rho_{CO2} = \frac{M_{CO_2}}{V_\varphi} \times 10^3$$

The CO2SOL keyword offers enhanced technical capabilities when it comes to solubility modeling compared to the other two simulation options. Moreover, if the reservoir contains an oil phase, it is capable of handling it with ease. Hence, this keyword can be considered a good alternative to the CO2STORE option in modeling carbon dioxide storage, even when the injection is happening into an aquifer.

2.4 GASSOL + SOLUHENRY Keyword

Lastly, the third simulation model under study in this project is the GASSOL keyword with the Henry solubility enabled through the SOLUHENRY keyword. It is an alternative method to CO2SOL, as it also involves an allowance for component solubility in the aqueous phase. However, not only does it enable more than one component to be dissolved in water, but it achieves it by utilizing fewer parameters and faster but with less detailed results. This simulation method is based on the three-phase, vapor-liquidwater equilibrium (tNavigator Simulation User Manual, 2024). In this case, the GASSOL keyword is paired with the SOLUHENRY, which indicates that the water phase solubility occurs per general Henry's law. Similarly, to the CO2SOL method, this approach also allows the definition of a solubility table through the SOLUBILI keyword; however, as previously discussed, in this study, the default solubility table was chosen to match the models by the number of moles injected with other parameters. Henry's law states that the partial pressure above a liquid is directly proportional to the amount of gas that is dissolved in that liquid; hence, it allows for the calculation of carbon dioxide solubility in the aqueous phase with the equation below:

$$f = xH$$

With f being the component volatility, x the fraction of CO2 in water, and H, the Henry's law constant, which can be calculated with the following expression:

$$ln(H) = ln(H_0) + v_\infty \frac{P - P_{ref}}{RT}$$

Here, R is the universal gas constant, H^0 represents the value of Henry's constant at the reference pressure and v_∞ stands for molar volume of water at infinite dilution. These parameters were first calculated using the default Li & Nghiem correlation. This method involves a series of calculations with a predefined table of coefficients and PVT data to come up with values for both H^0 and v_∞ [22]. However, these values were modified manually to maintain compliance with other models in this study regarding the molar volume of injected carbon dioxide during the injection period. The GASSOL model with Henry's law enabled has its most significant advantage in reducing used parameters compared to the other models considered. Therefore, on paper, it could appear an excellent candidate to utilize during large-scale projects requiring tons of computational power.

2.5 Simulation Parameters and Scenarios

Each model has been injected with the same stream of pure, supercritical CO_2 at the same rate - 3,000 Mscf/day. Such injection was set to last three years, followed by a 100-year-long well shut-in period, during which the distribution of carbon dioxide plume was studied. During the injection period, the data in the simulator was collected weekly and every five years during the shut-in. Additionally, each calculation method was capped by a reservoir pressure of 8,700 psia. If this pressure was reached, the injector well was supposed to shut-in until the pressure dropped below the specified value. Such a restriction was imposed on all models. However, it was introduced due to the technical specification of the CO2STORE keyword that does not allow reservoir pressure to exceed 8,700 psia during the injection period. All the injection parameters can be found in Table 3, provided below.

Parameter	Value	Unit
Injection Rate	3,000	Mscf/day
Injector Well Diameter	0.625	ft
Top of Perforations	5,000	ft
Bottom of Perforations	5,400	ft
Injector Well Grid Placement (x, y)	(637.5, 637.5)	(ft, ft)
Maximum Injection Pressure	8,700	psia
Injection Period	3	years
Shut-in Period	100	years
Reservoir Fluid	pure H_2O	
Injected Fluid	pure CO_2	

Table 3: Injection Parameters Used in all Models within this Project.

Relative permeability curves have been obtained from the Illinois Basin - Decatur Project's injection model. In that case, the values remained realistic since the data was modeled after a real-world CO_2 storage project. However, the curves were converted to a power-law through the method presented by Corey in 1954. This allowed us to decrease the computation times considerably.

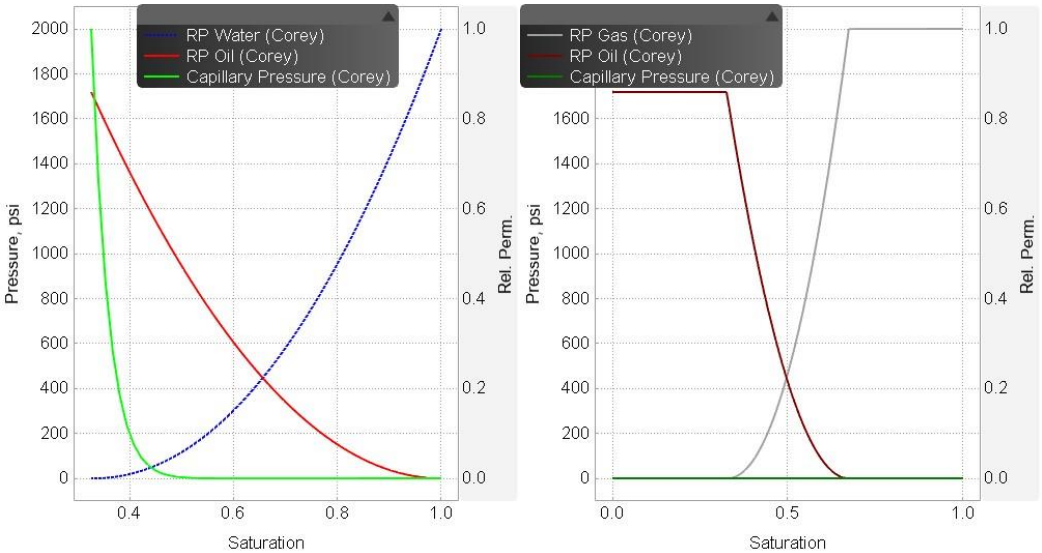

Figure 1: Relative Permeability Curves from the IBDP Project Utilized in this Study.

Each model included an element of variability in the form of the grid size change. Each calculation method involved running six separate simulations; the only difference between them was the number of cells within the same-sized rectangular prism. It started from as little as 11,560 cells, decreasing the cell size by 7.5 ft steps until 416,160 cells were reached. This procedure allowed us to not only compare the different keywords against each other but also to factor in the grid as a variable since all three models have a different set of governing equations that vary in complexity. Therefore, the grid size plays a more significant role in the calculation time and the accuracy of these calculations.

cell length	cell width	cell depth	grid dimensions	number of cells
12.5 ft	12.5 ft	10.0 ft	102 x 102 x 40	416,160
25.0 ft	25.0 ft	10.0 ft	51 x 51 x 40	104,040
37.5 ft	37.5 ft	10.0 ft	34 x 34 x 40	46,240
50.0 ft	50.0 ft	10.0 ft	26 x 26 x 40	27,040
62.5 ft	62.5 ft	10.0 ft	21 x 21 x 40	17,640
75.0 ft	75.0 ft	10.0 ft	17 x 17 x 40	11,560

Table 4: Grid Sizes in question and their Parameters.

3. Results and Discussion

The objective of the carbon storage process, as the name suggests, is to store carbon dioxide, in this case, within an aquifer. Each simulation variant injected a similar number of moles into the reservoir
(approximately 8,665 thousand pound-mole each). Due to differences in the technicalities of each model, the process of storing the CO_2 looked slightly different. This section of the study will go in-depth into analyzing these differences. Moreover, the differences in geometry of the overall sizes of the CO_2 plumes between the simulation methods were questioned. Additionally, each model was subject to a sensitivity analysis to determine whether at all or how big of an effect the size of an individual cell can have on the dissolution mechanisms and the plume size.

3.1 Number of Moles of CO_2 Mobile in Gas

For each model, the number of carbon dioxide moles mobile in gas steadily increases until the end of the injection period; however, it does so at different rates. As shown in the graph below, the highest number of moles of CO_2 is mobile in gas in the CO2STORE model, whereas the two other models are behind by at least a factor of 3. Throughout the shut-in period, this statistic decreases for all three models until there is no mobile gas left. That indicated that the plumes have developed and settled in place in all cases.

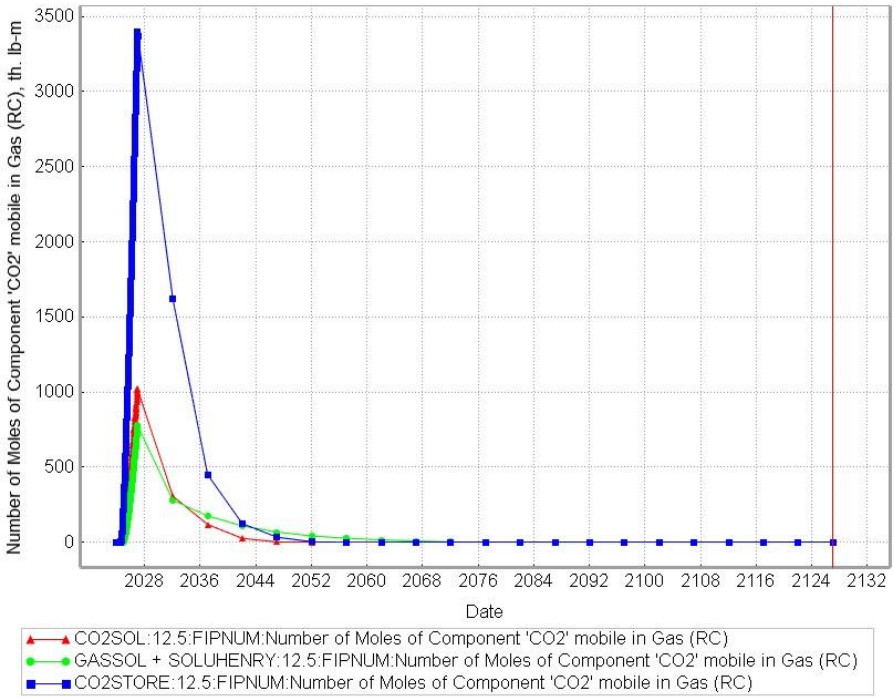

Figure 2: The Comparison of the number of moles of CO_2 mobile in gas vs. Time Between the Simulation Methods.

What is worth mentioning is that despite the most significant number of moles of mobile CO_2 in gas after the injection period, the CO2STORE model reaches zero the fastest. This is caused by the most efficient, by default, dissolution mechanism utilized in this approach. Oppositely, the GASSOL keyword with Henry solubility enabled is the last model achieving no mobile carbon dioxide in the gaseous phase, even though it had the smallest number at the start of the shut-in. Above all, this graph proves that the one hundred years period is sufficient to prevent the CO_2 plume from further movement.

3.2 Number of Moles of CO_2 Trapped in Gas

When analyzing the number of carbon dioxide moles trapped in gas, the first thing that must be mentioned is that the default dissolution mechanism used by the CO2STORE keyword did not allow for any CO_2 trapping in the gaseous phase. In other words, the injected supercritical fluid could dissolve fully without being trapped in gas, as can be seen on the graph below; neither of the two methods reached zero, indicating a defined carbon dioxide plume within the reservoir.

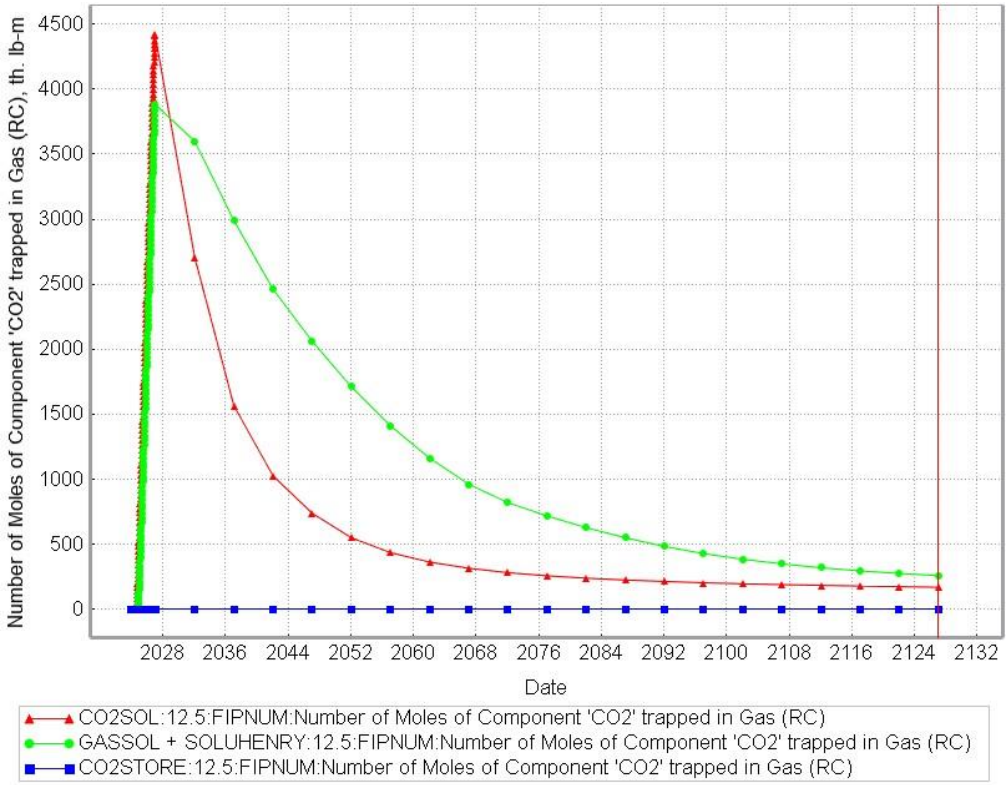

Figure 3: The comparison of the number of moles of CO2 Trapped in gas vs. Time Between the Simulation Methods.

Interestingly, the CO2SOL simulation started with a more significant number of CO_2 moles trapped in gas than the GASSOL version. However, the latter is characterized by a slower dissolution mechanism; hence, by the end of the shut-in period, the plume had a larger number of moles than the CO2SOL version. Figure 2 displays the respective plumes at different stages throughout the shut-in period. Carbon dioxide migration due to gravity within the aquifer can be easily seen, and the dissolution process results in the decreasing volume of the plume.

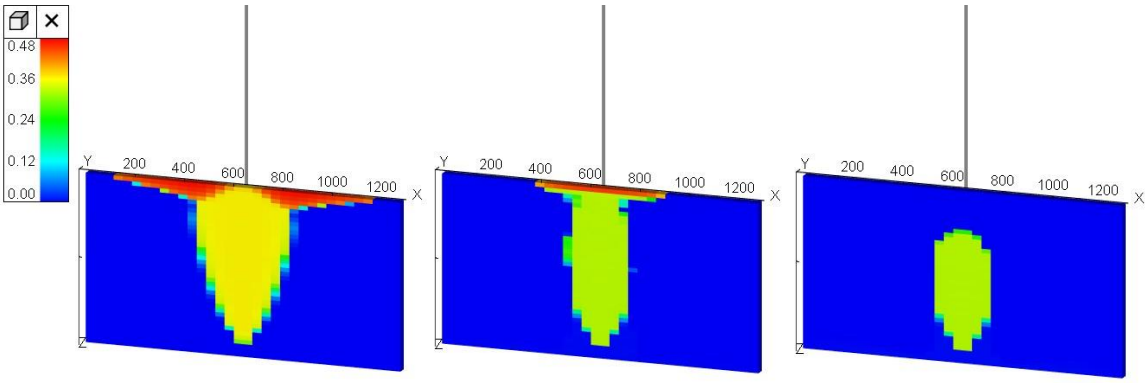

Figure 4: The Evolution of the Positioning and Volume of the Carbon dioxide plume over the Course of the Shut-in.

3.3 Number of Moles of CO_2 in Water

The effect of the previous two statistics can be seen in the graph representing the number of carbon dioxide moles in water. Since all three simulations do not contain an oil phase, the injected supercritical CO_2 can either be mobile, trapped in gas, or dissolved in water. Therefore, the phenomena seen in the first two are reflected in the numbers presented in Figure 5 below.

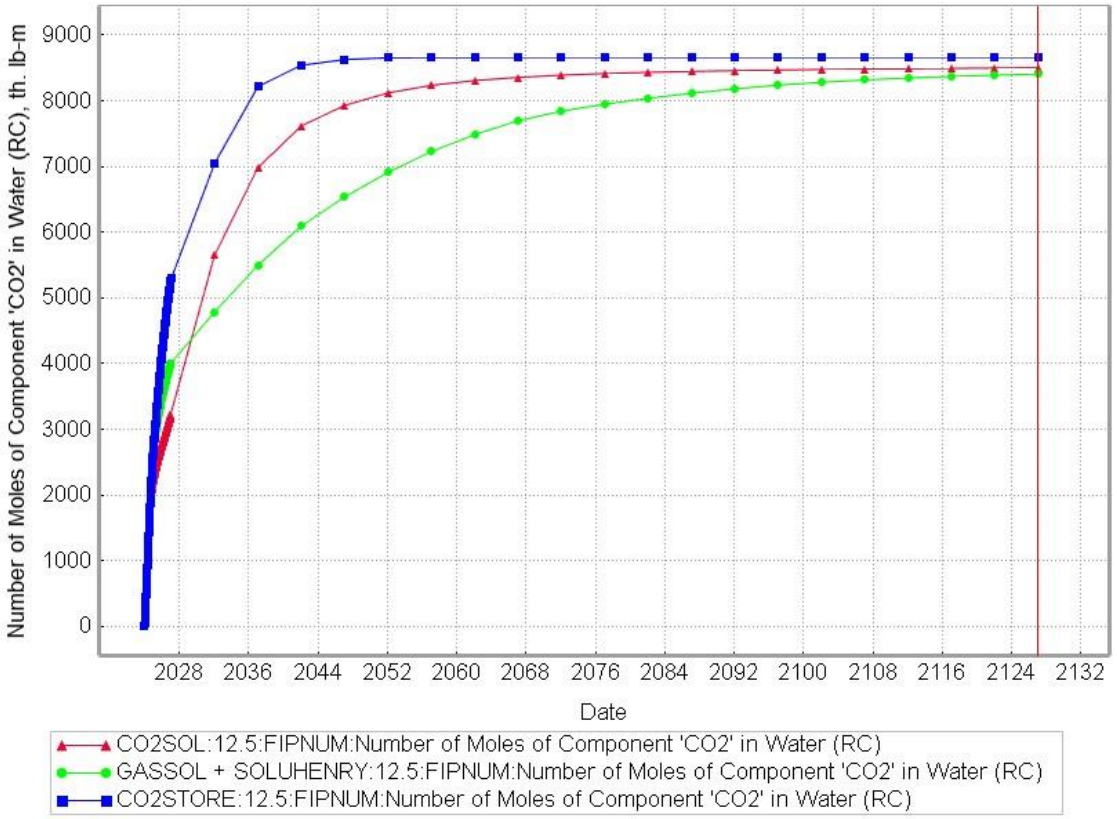

Figure 5: The comparison of the number of moles of CO2 in waters. Time between the Simulation Methods.

The lack of mobile CO_2 in the gaseous phase of the CO2STORE and its fast dissolution mechanisms can be easily spotted as the number of moles in water reaches the plateau the fastest among the simulations in this study. The slowest dissolution and the largest carbon dioxide plume of all models are shown, and the GASSOL curve visibly "lags" behind the other two while never truly reaching a visible plateau. What is interesting to see is that the curves do not separate from one another in the slightest until late August - over eight months into the injection period. Only after the data point 09/02/2024 does the CO2SOL simulation fall behind regarding the number of carbon dioxide moles in water.

3.4 Plume Size Analysis

Plume migration analysis is an essential aspect of every carbon

storage project. A simulation's ability to accurately model the size and movement of the trapped CO_2 is a greatly desired feature. This study does not answer the question of whether one model calculates the migration mechanisms better than others; however, it was able to investigate the general trend and behavior of the plume in each model to possibly help determine the correct option for a specific application. Firstly, this project's goal was to determine the differences in the carbon dioxide dispersion mechanisms within the rock matrix during and right after the injection. For this project, 2D maps were created for each model, which represent average gas saturation in each cell on the day the injector well was shut. Figures 6, 7, and 8 show that the curves regarding the number of moles in each phase represent the plume. Firstly, this project's goal was to determine the differences in the dispersion mechanisms of the carbon dioxide within the matrix of the rock during and right after the injection. For the purposes of this project, 2D maps were created for each of the models, which represent average gas saturation in each cell on the day that the injector well was shut. Figures 6, 7, and 8 allow to see that the curves regarding the number of moles in each phase have a representation on the plume.

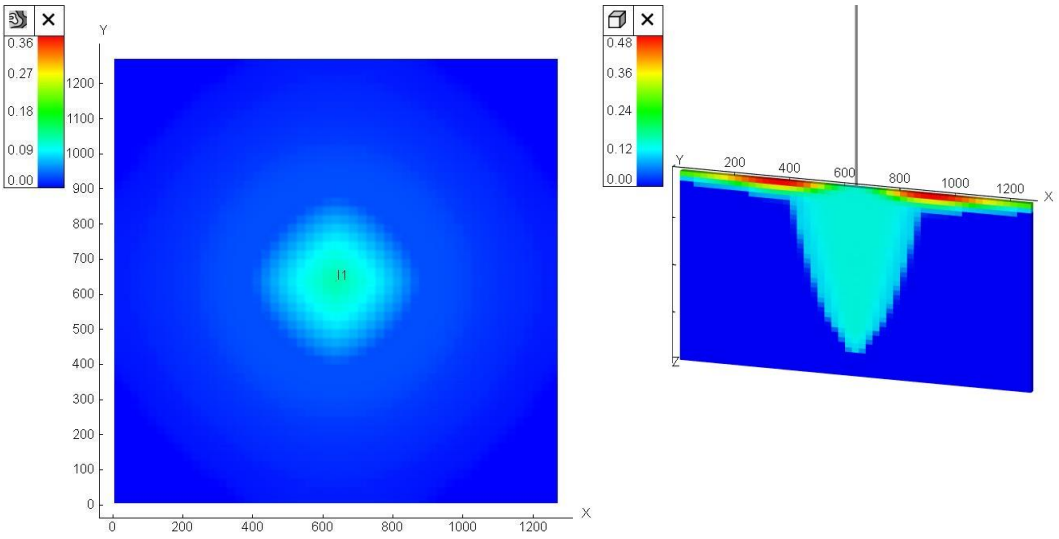

Figure 6: Gas saturation on a 2D-map and a cross section of the reservoir of the CO2STORE model at the end of the injection period.

In the case of the CO2STORE model, one can see that the solubility of carbon dioxide in the water greatly affected the gas saturation and, consequently - the formation of the plume. Besides the scale that indicates lower gas saturation values, the results look similar to the remaining two. However, a phenomenon has already been observed during reservoir modeling of carbon dioxide storage in the Sleipner gas field in Norway [25]. While using CO2STORE, injected CO_2 tends to occupy a limited space at the top of the aquifer despite the perforations occurring throughout the entirety of the mode. This happens due to a significant density difference between the supercritical carbon dioxide and the reservoir fluid. Hence, CO_2 continues to spread underneath the non-permeable ceiling of the grid laterally [26].

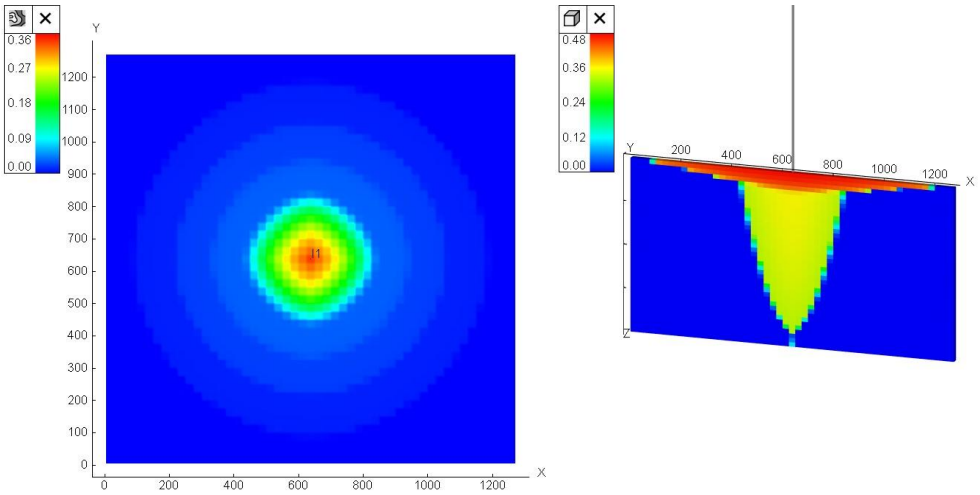

Figure 7: Gas saturation on a 2D-map and a cross section of the reservoir of the GASSOL + SOLUHENRY model at the end of the injection period.

The GASSOL + SOLUHENRY model exhibits a very predictable behavior in which the carbon dioxide in the gaseous phase is located at the very top of the aquifer. In contrast, the dissolved CO_2 begins to slowly sink to the bottom of the reservoir due to its increased density. The injected fluid does spread laterally to some extent, primarily due to less carbon dioxide being dissolved in water quickly enough.

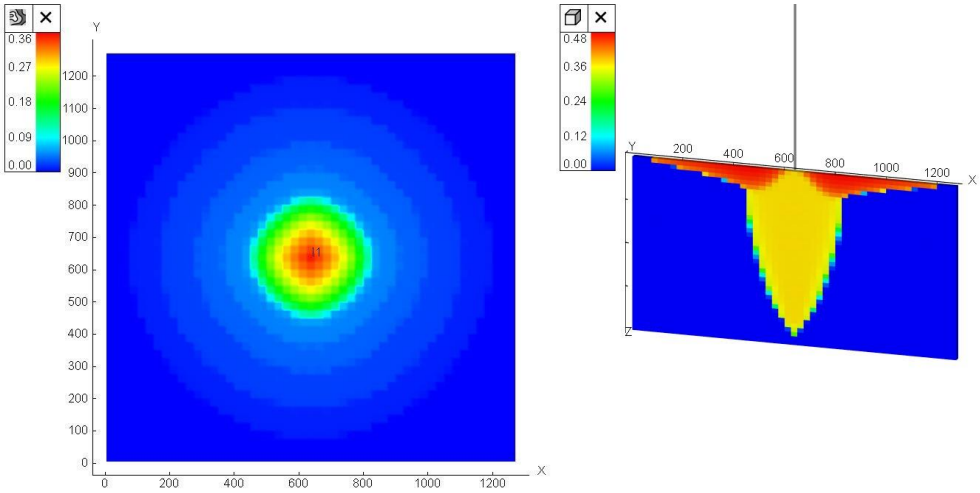

Figure 8: Gas saturation on a 2D-map and a Cross Section of the Reservoir of the CO2SOL Model at the end of the Injection Period.

When it comes to the CO2SOL model, the enhanced solubility of the carbon dioxide can be seen as the cross-section indicates that there is more of the injected component around the vicinity of the wellbore and less at the top of the reservoir. Also, despite the same injection rate across the three models, the 2D map of the CO2SOL model shows that there is a larger concentration of carbon dioxide within a small radius of the injector. As mentioned earlier, the CO2STORE keyword does not produce a gaseous plume as the entirety of the carbon dioxide dissolves into the reservoir water throughout the hundred years of shut-in. Hence, there are only two models to consider when it comes to plume size post-shut-in. The graphs describing the number of moles of carbon dioxide also allow us to predict the behavior of the plumes here. The Henry solubility option, characterized by slower dissolution, leads to a larger volume of CO_2 compared to the CO2SOL option. This is a key factor in the behavior of the plumes. The deepest point of the plume occurs at the same depth as the one in the other model; however, the trapped gas extends higher into the aquifer as well as to a greater radius.

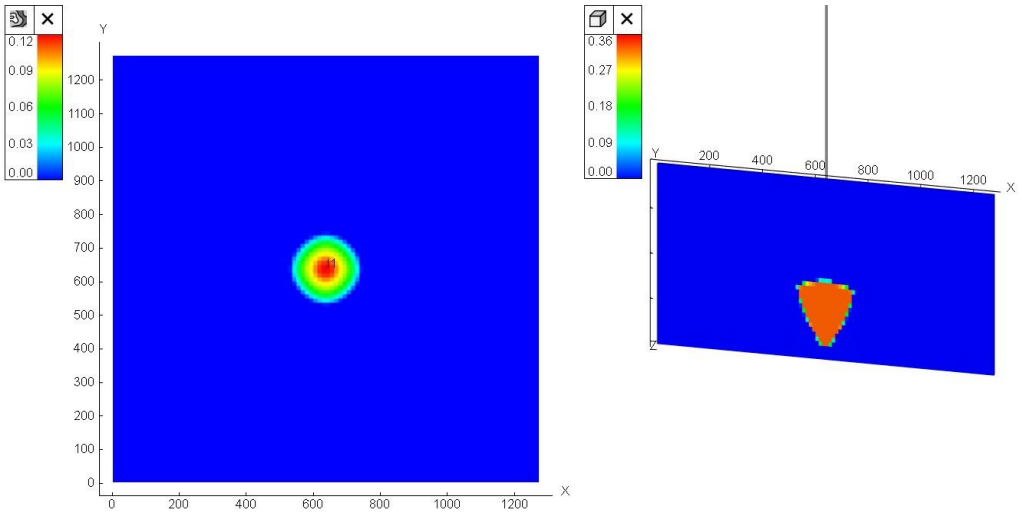

Figure 9: Gas saturation on a 2D-map and a Cross Section of the Reservoir of the GASSOL + SOLUHENRY Model at the end of the Shut-in Period.

By the end of the shut-in period, both plumes appeared to be stationary. The dissolution processes would most likely still occur but to a much smaller extent. In the last 15 years of the simulation, the parameters of the CO2SOL model remained unchanged, whereas in the GASSOL model, the differences were noticeable yet insignificant in scale.

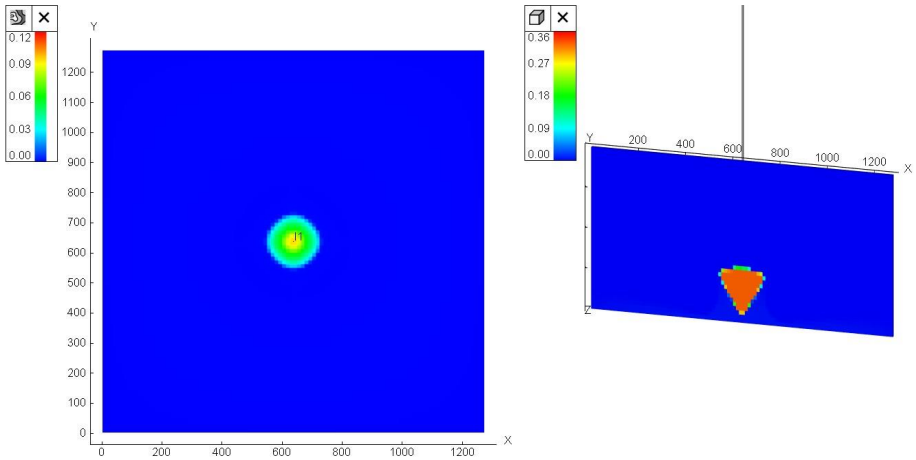

Figure 10: Gas saturation on a 2D-map and a Cross Section of the Reservoir of the CO2SOL model at the end of the Shut-in Period.

3.5 The Effect of the Grid Size on the Plume Area

Grid size is one of the most important parameters when running a numerical simulation. Such a model works based on the principle that before moving on to the next cell, certain conditions must be fulfilled in the active cell. These conditions vary based on the model and application; however, the idea is that the larger the block, the more it will take to meet a given criteria. Moreover, the lower the number of cells, the greater the chance that the model will either overestimate or underestimate the actual value. A solution to this problem would be to infinitely increase the number of blocks. Unfortunately, the higher the number of cells, the more computational power it takes to carry out the required calculations. In this study, the grid size was varied to investigate the scale of differences between the plume areas. This was done in the hope of finding a reasonable grid size with respect to computational time and accuracy. The table below contains values of the calculated area of the trapped gas in GASSOL + SOLUHENRY and CO2SOL models with the corresponding choice of grid dimensions.

grid dimensions	plume area after 100 years	
X x Y x Z	CO2SOL, ft^2	GASSOL, ft^2
102 x 102 x 40	25,226	33,142
51 x 51 x 40	20,278	26,944
34 x 34 x 40	28,281	28,281
26 x 26 x 40	17,778	24,444
21 x 21 x 40	12,153	12,153
17 x 17 x 40	17,500	12,153

Table 5: A summary of the plume size differences caused by the changes in the grid size.

The criteria for classifying an active cell into the plume was that it had a value of gas saturation greater than 1%. This allowed us to sieve the cells that would drastically increase the area while simultaneously overestimating the actual results. Table 5 indicates that the finest grid, statistically the closest to the real solution, approximates the plume area between 25,226 and 33,142 square feet. A one-step, coarser grid provides a lower value that most likely underestimates the proper area. However, through a series of underestimates and overestimates, the 15 ft coarser grid is surprisingly close to the solution provided by the model utilizing the finest grid. One could say that choosing the 34 by 34 by 40 grids is the optimal solution for this scenario. However, upon investigating the actual 2D maps, it is trivial to see that the result close to the original solution is a product of coincidence above anything else.

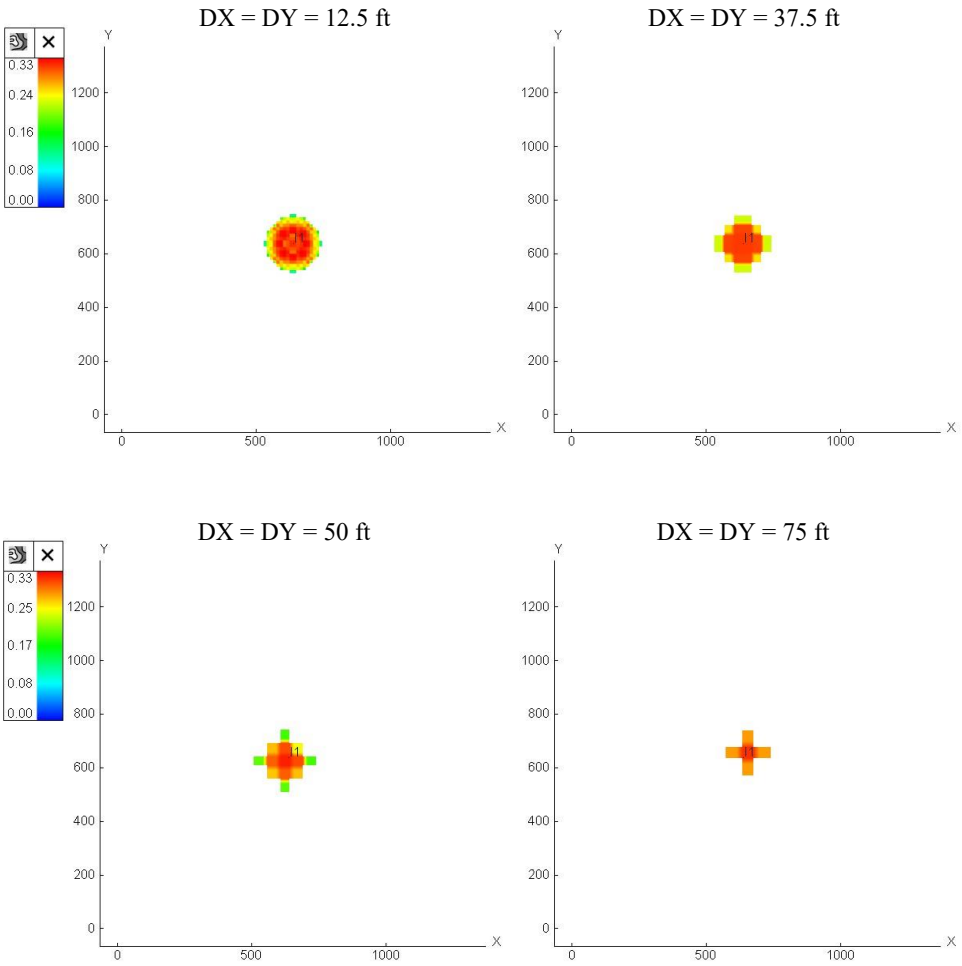

Figure 11: The Differences in Plume area Approximation with Respect to Cell Size.

3.6 The Effect of the Grid Size on the Injection Parameters and Results

As each block is a separate set of calculations, the size of it could potentially impact the results of the injection phase just as it did affect the carbon dioxide dispersion within the rock matrix. Upon checking the graphs and tables with the results of the simulation, for all three models, the results were so close to each other that the slight differences between the values were most likely caused by the nature of the calculations governing the simulations. Therefore, the grid size was deemed insignificant regarding the injection parameters and results.

3.7 The Effect of the Calculation Method and the Grid Size on the Simulation Run Time

Altering cell dimensions while maintaining the overall grid volume can exponentially affect the total number of cells in the model. In this study, the length and width of the blocks were altered by a factor of 7.5 ft. The smallest length and width equal 12.5 ft, with 75 ft being the largest. As a result, the number of cells in the simulation was increased by a factor of 36. Such a dramatic increase intuitively must lead to increased simulation time. Depending on the model, the simulation time was increased 168 times. However, one must point out that the step from 25 ft in width and length down to 12.5 ft leads to the most significant linear increase in time, which can make such a decrease a questionable choice, especially when we consider the minor differences in the plume area results and virtually no differences in the injection calculations that were discussed in the previous sections.

grid dimensions	number of cells	CO2STORE	CO2SOL	GASSOL
102 x 102 x 40	416,160	8h 12min 13s	4h 34min 08s	3h 45min 55s
51 x 51 x 40	104,040	1h 08min 07s	1h 10min 18s	1h 03min 47s
34 x 34 x 40	46,240	18min 45s	6min 32s	6min 33s
26 x 26 x 40	27,040	12min 20s	3min 04s	5min 37s
21 x 21 x 40	17,640	6min 35s	1min 57s	2min 08s
17 x 17 x 40	11,560	4min 08s	1min 38s	1min 35s

Table 6: The Effect of the Grid Size and the Model Variant on the run time of a Simulation.

4. Conclusions

This study rigorously evaluated the effects of grid size and simulation methodologies on modeling supercritical CO2 injection and storage in aquifers. This project utilized tNavigator software with
CO2STORE, CO2SOL, and GASSOL+SOLUHENRY simulation strategies. Key findings include the influence of the grid size on the simulation's accuracy and computational demand and the necessity for an optimal balance, which is crucial to achieving reliable results. Among the methodologies, CO2STORE demonstrated superior efficacy in CO_2 dissolution. It emphasizes the importance of selecting a method based on the specific characteristics of the geological storage site.

This research provides practical insights into the complex interplay between simulation parameters and their impact on the modeling of geological carbon storage. These insights can be leveraged to enhance the accuracy and efficiency of carbon sequestration simulations. It is a crucial aspect of our collective efforts to combat climate change. Moreover, this study encourages future research to explore integrating dynamic geological features and alternative modeling techniques, which could further advance the carbon capture and storage field as a viable solution to climate change.

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