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## **Upscaling of Diffusivity in CO<sub>2</sub> Storage Processes in Deep Saline Aquifers**

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### **Abstract**

Anthropogenic greenhouse gas (GHG) emissions, particularly carbon dioxide (CO<sub>2</sub>), have been rising drastically, contributing to climate change. One of the key potential solutions to mitigate the rising CO<sub>2</sub> concentrations in the atmosphere is to capture and store CO<sub>2</sub> (CCS) in underground geological formations, such as depleted oil and gas reservoirs or deep saline aquifers.

Saline aquifers are considered to be important in terms of their substantial capacity for CO<sub>2</sub> storage and their extensive availability which can play an important role in source and sink match leading to reduced transportation costs. Injection and storage of CO<sub>2</sub> in such systems is governed by various physical and chemical processes leading to retaining and trapping the CO<sub>2</sub>. Among the various trapping mechanisms, this paper highlights solubility (dissolution) trapping. While solubility trapping is a slower process (in the context of injection timescale) compared to structural/stratigraphic and residual trapping, it offers more stable and reliable storage in the timescales aligned with the storage time. The dissolution of CO<sub>2</sub> into the aqueous phase, followed by its eventual sequestration as carbonates, enhances the permanence and security of storage. Denser CO<sub>2</sub>-brine mixture at the top emanating from the CO<sub>2</sub> plume creates gravity-based instabilities in the system, leading to density-driven fingering that triggers downward movement and speeds up CO<sub>2</sub> dissolution via local mixing.

This study investigates the impact of grid size on CO<sub>2</sub> dissolution, diffusion, and convection in brine using high-resolution numerical simulations based on diffusivity measurements in our laboratories. The pressure decay technique used for measurements under high pressure, temperature, and salinity conditions provided the experimental data for developing a realistic model that accurately captures the effective diffusivity on dissolution in a bulk media at a reservoir scale. Several commercial simulators were tested, with metrics including pressure and CO<sub>2</sub> dissolution as a function of time, as well as CO<sub>2</sub> concentration at depth intervals.

The preliminary results indicate that all simulators used in this study reflected grid size effects to some extent. The pressure decay predicted by the model closely matched the experimental base case, validating the model and increasing confidence for the next stage of this study. The findings of this research offer valuable insights into the design and risk mitigation of CO<sub>2</sub> storage projects.

## Introduction

Greenhouse gas (GHG) emissions remain an environmental concern as emissions have led to global warming by trapping heat energy in the atmosphere and slowing down the rate at which the energy escapes into space (Mohajan, 2011; Kweku et al., 2018; US EPA, 2024). CO<sub>2</sub> has the most impact on all GHGs due to its relatively longer lifespan and abundance in the atmosphere. Reducing CO<sub>2</sub> emissions is of utmost importance in order to meet the Paris Agreement target of global temperature increase to 1.5 °C above pre-industrial levels (United Nations, n. d.).

Various technologies have been proposed to reduce GHG emissions, one of which is storage in geologic formations, including oil and gas fields, saline aquifers, coal seams, basalts, oil and gas-rich shales, and salt caverns (Paker et al., 2025; Dindoruk and Livescu, 2023; Khan et al., 2023; Magzymov et al., 2022). Deep saline aquifers are desirable due to their widespread availability and large capacities (Celia et al., 2015).

The containment and safety of injected CO<sub>2</sub> in underground formations are crucial for the success of CCUS. CO<sub>2</sub> is usually injected in a supercritical state (temperature = 31.04 °C, pressure = 73.82 bar) at depths of greater than 800 m, thereby maximizing the storage capacity. Various trapping mechanisms secure the injected CO<sub>2</sub>, including structural trapping, residual trapping, mineral trapping, and solubility trapping (IPCC, 2005; Han et al., 2010; Iglaur, 2011; Szulczewski et al., 2013; Zhang and Song, 2013; Benavides et al., 2023). The diffusion coefficient is an important parameter for modeling CO<sub>2</sub> storage in the aquifer. It ensures accurate capturing of the dissolution process and prediction of the evolution of CO<sub>2</sub> over time and will control the onset and development of connective instabilities (Teng et al., 1997; Riaz et al., 2006; Azin et al., 2013; Omrani et al., 2021). Moreover, when unreliable diffusivity data is used, numerical models may underestimate or overestimate trapping potential, leading to inaccurate assessments of storage performance and safety.

Field-scale simulation is used to determine the spread of the injected CO<sub>2</sub> and monitor it for leakages. It is fast becoming the leading approach for predicting subsurface storage. (Massarweh and Abushaikha, 2024; Benevides et al., 2024). Grid resolution plays a crucial role in accurate CO<sub>2</sub> storage predictions in saline aquifers using numerical simulation. Too large grids will underestimate the quantity of CO<sub>2</sub> stored (Suriano et al. 2022; Likanapaisal et al. 2023), underestimate the dissolution rate, and vertical migration while underestimating pressure decline due to dissolution Ismail et al. (2024). Studies recommend using fine grids for reliable predictions, especially during the early storage phases, with grid size selection carefully balanced to optimize accuracy and computational efficiency (Ismail et al., 2024; Lichtner 2007; Suriano et al., 2022). Various authors studied the effect of grid resolution on accurate modeling of storage behavior during the monitoring phase simulation. Still, to the best of our knowledge, none compared the same parameters on various well-known simulators and compared the results to ensure that the selected grid sizes are applicable to multiple simulators. Furthermore, none used the recommended grid sizes to match the pressure decay data from experiments.

In this study, we investigated the influence of grid resolution and upscaling techniques on CO<sub>2</sub> dissolution, diffusion, and convection in brine through the use of high-resolution numerical simulations. We use CO<sub>2</sub> diffusivity in brine data obtained from pressure decay experiments at suitable aquifer conditions of high temperature (T), pressure (P), and salinity (S) range (p= 1400 psi, T= 60°C and S= 15,000, 50,000, 100,000, and 200,000 ppm) to develop realistic models to capture diffusivity at the reservoir scale. We evaluated multiple commercial simulators, focusing on key metrics such as pressure evolution, CO<sub>2</sub> dissolution rates over time, and concentration profiles at various depth intervals, ensuring a comprehensive analysis of the processes.

## Methodology

In this study, we used data obtained from pressure decay experiments to validate theoretical analyses and numerical models. Another study by Oyagha et al. (2024) provides more details related to experimental work and theoretical analysis. The theory of the mathematical model, including governing equations used in simulations, was explained in detail here.

## Experiment setup and procedure

Pressure decay experiments are run based on the methods presented in detail in (Oyagha et al., 2024.; Ratnakar and Dindoruk, 2015; 2019; 2020; 2022; Ratnakar et al., 2019; Riazi, 1996; Zhang et al., 2000; Sheikha et al., 2005). The experiment setup is shown in Figure 1. The system is leak tested using nitrogen for up to 24 hours to ensure all pressure changes in the system are from dissolution. All cells are vacuumed for about 30 minutes to remove any contaminating gases. The liquid and gas cells are filled with brine and CO<sub>2</sub>, respectively, and kept in the oven for 24 hours to heat up to the test temperature. A known volume of liquid is injected into the experiment cell, and then gas is injected up to the test pressure. All valves are closed, and the pressure changes with time is recorded while monitoring the temperature to ensure an isothermal system.

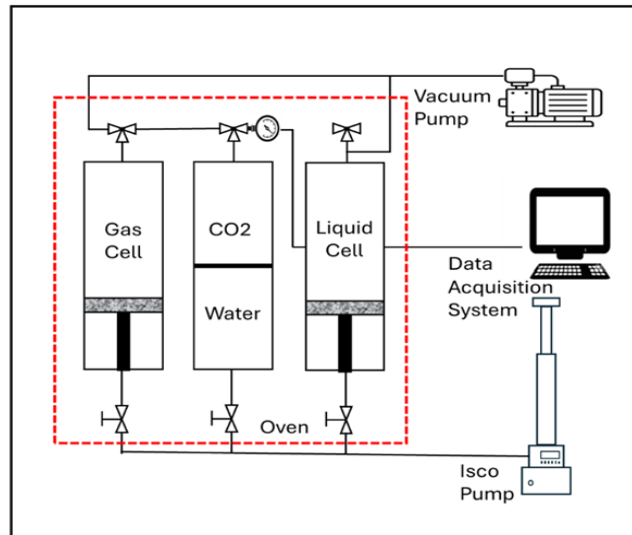


Figure 1- Pressure Decay Experiment Set-up (Oyagha et al., 2024).

## Numerical model description

### Governing equations

The governing equations for convective mixing include the continuity equation and the mass balance equation. The continuity equation in the porous medium is given by

$$\frac{\partial(\phi_m \rho)}{\partial t} = -\nabla \cdot (\rho u) \quad (1)$$

where  $t$  is the time,  $\phi_m$  is the matrix porosity,  $\rho$  is the mixture density, and  $u$  is Darcy's velocity. Fluid density is a function of temperature, pressure, and component concentration. The density equation expressed by Diersch and Kolditz (2002) is used for simplicity.

$$\rho = \rho_0 \left[ 1 + \sum_{i=1}^n \beta_i (c_i - c_{0,i}) \right] \quad (2)$$

$$\beta_i = \frac{1}{\rho_0} \left[ \frac{\partial \rho}{\partial c_i} \right]_T \quad (3)$$

Where  $\rho_0$  is the density of CO<sub>2</sub>-free water,  $\beta_i$  is the densification coefficient.

### Boundary and initial conditions

The domain boundaries are characterized to govern the flow and concentration behaviors. For the left, right, and bottom boundaries, impermeability is assumed, resulting in the following conditions:

$$u_x(0, z, t) = u_x(W, z, t) = u_x(x, H, t) = 0 \quad (4)$$

$$\left[ \frac{\partial c}{\partial x} \right]_{x=0} = \left[ \frac{\partial c}{\partial x} \right]_{x=W} = \left[ \frac{\partial c}{\partial z} \right]_{z=H} = 0 \quad (5)$$

At the top boundary, a constant pressure condition is implemented to satisfy the continuity equation:

$$c(x, 0, t) = 1 + A_0 \sin(2\pi x / \lambda_0) \quad (6)$$

To account for perturbations caused by CO<sub>2</sub> injection or formation heterogeneity, a sine wave function is introduced. This function represents the concentrations of CO<sub>2</sub> at the top boundary and is defined as

$$c(x, 0, t) = 1 + A_0 \sin(2\pi x / \lambda_0) \quad (7)$$

Where  $A_0$  is the dimensionless amplitude of the sine wave function and  $\lambda_0$  denotes the wavelength. Initially, the water phase contains no CO<sub>2</sub>, and the pressure in the domain is equal to the pressure at the top boundary:

$$c(x, z, 0) = 0 \quad (8)$$

$$P(x, z, 0) = P_{top} \quad (9)$$

### Model setup and simulation parameters

To investigate the density-driven convection, a two-dimensional domain system was built using COMSOL Multiphysics 5.5. Where the top layer represents the CO<sub>2</sub> supercritical domain, and the bottom layer is the free-CO<sub>2</sub> saturated brine domain. The dimensions of width and height of both domains were 10 cm to honor the dimensions of the experimental setting. The brine in the research domain has varying salinities (refer to Table 1) and no gas was initially dissolved. All domain boundaries were assumed to be closed, and the pressure decay on the CO<sub>2</sub> domain was modeled to match the experimental data. Other assumptions included the following: First, no porous media was assumed, therefore the two-phase transition zone caused by capillary pressure was ignored. Second, the domains were assumed to be isothermal. The initial CO<sub>2</sub> density and viscosity calculated using the correlations from Dindoruk et al. (2022) are 1125.9 kg/m<sup>3</sup> and 1.7e-4 Pa\*s respectively.

Table 1. Simulation parameters.

Parameter	Value	Units
<i>Temperature</i>	60	°C
<i>Initial pressure at the top boundary</i>	1400	psi
<i>Salinity</i>	15,50,100 & 200 k	ppm
<i>Matrix porosity</i>	1	v/v
<i>Matrix permeability</i>	1000	mD
<i>Amplitude of sine function (<math>A_0</math>)</i>	0.01	-
<i>Wavelength of sine function (<math>\lambda_0</math>)</i>	1/12	-

To simulate the convective dissolution problem in COMSOL, the “Darcy’s flow” interface and the “transport of diluted species in porous media” interface were coupled. To accurately capture the diffusive behavior during the early stages, it is necessary to ensure that the grid size near the top boundary is smaller than the critical thickness of the diffusive boundary layer at the onset of convection. In this study, a grid sensitivity analysis is carried out to investigate the numerical effect caused by grid discretization. Three grid settings are investigated, a fully rectangular grid with a resolution of 0.1 cm, a triangular grid with a resolution of 0.1 cm, and a local grid refinement (LGR) at the top boundary. This last grid setting has a

gradual grid size increment away from the top boundary from 0.01 cm, the grid block size gradually increased from 0.1 cm to 0.4 cm in order to capture the fingering at the transition zone and to improve computational efficiency.

**Results**

**Grid sensitivity analysis**

To investigate the numerical effect caused by the grid shape and size. The CO<sub>2</sub> fingers in a 100k ppm brine after 24 hours showed a significant symmetrical difference among the grid cases. Figure 2a shows the difference quantitatively where the maximum saturation is reached at 24 hours. The local grid refinement shows the highest saturation due to the higher concentration of small grid at transition zone which generates higher saturation of CO<sub>2</sub> close to the top boundary. Due to the larger grid size the numerical averaging is larger causing a higher prediction of CO<sub>2</sub> saturation at the end of the simulation time (refer to Figure 2b).

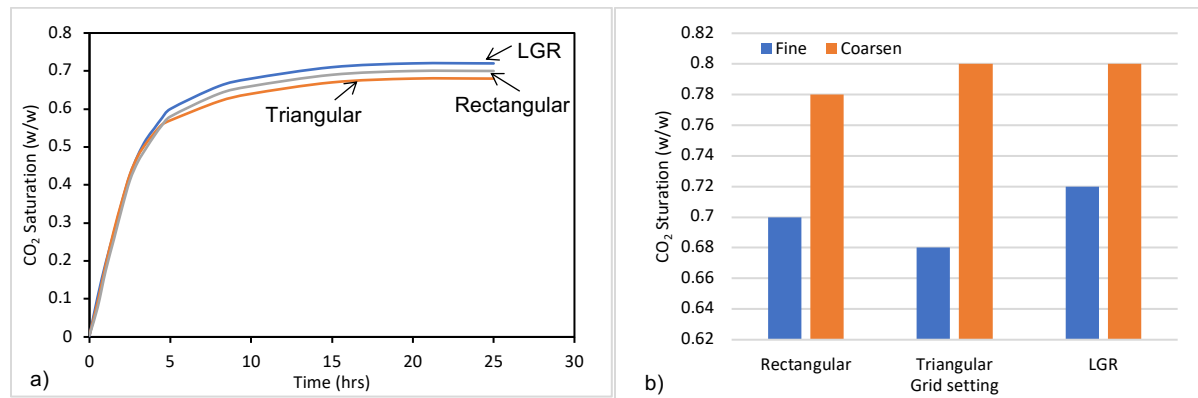


Figure 2 — a) Comparison of the evolution of CO<sub>2</sub> saturation in brine among the different grid settings, b) Comparison of CO<sub>2</sub> saturation in brine among the different grid resolutions and grid settings.

**Model calibration and validation**

The reliability of the numerical model is assessed using data from a published study where the diffusion coefficient of methane in hexadecane was experimentally measured (Dindoruk et al., 2023). The diffusion coefficient obtained by Sherry et al. (2024) is  $2.15 \times 10^{-9}$  m<sup>2</sup>/s, which closely aligns with the  $2.32 \times 10^{-9}$  m<sup>2</sup>/s reported by Dindoruk et al. (2023). The experimental pressure decay serves as an indicator of the numerical model's performance. Figure 3 demonstrates that the pressure decay in the CH<sub>4</sub> domain predicted by the numerical simulator agrees with the experimentally measured data, indicating that the numerical model accurately captures the behavior in the top layer.

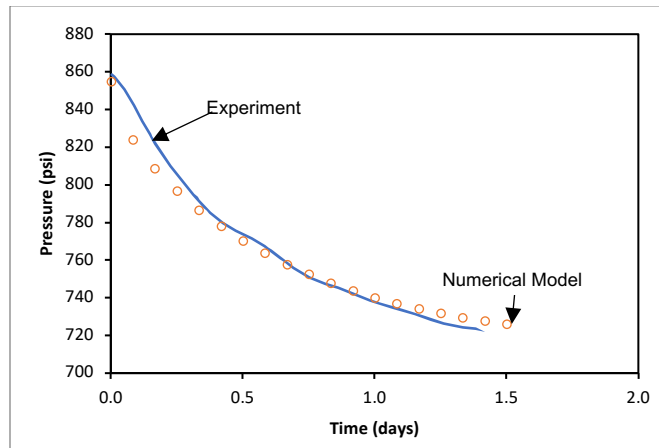


Figure 3 — Comparison between the experimental and numerical model pressure decay in the Methane domain.

A detailed analysis of the numerical model revealed that the diffusivity and the concentration of the dissolved species were back-calculated the analytical solution to Fick's second law for a constant surface concentration is:

$$\frac{c_s - c(x,t)}{c_s - c_0} = \operatorname{erf}\left(\frac{x}{2\sqrt{Dt}}\right) \quad (10)$$

Where  $c_s$  represents the surface concentration where a single species is present ( $\text{CH}_4$  or  $\text{CO}_2$ ), and  $c_0$  is the initial concentration of the dissolved species in the solvent domain, which in this study is zero. The term  $\operatorname{erf}\left(x/2\sqrt{Dt}\right)$  is the error function that describes the relationship between depth ( $x$ , in meters) and the square root of the diffusivity coefficient ( $D$ , in  $\text{m}^2/\text{s}$ ) divided by time ( $t$ , in seconds).

Using Equation 10, the concentration profile is back-calculated based on the diffusivity value reported from the laboratory experiment and compared to the concentration profile obtained from the numerical model. Figure 4a shows the  $\text{CH}_4$  concentration profile in the hexadecane domain at three different times (2, 18, and 36 hours). A good agreement is observed between the concentrations calculated from the numerical model and the analytical model. A closer inspection revealed that the numerical model is sensitive to very low concentrations (early stages), leading to a slight overestimation of the analytically calculated diffusivity coefficient (see Figure 4b). The difference between the numerical model diffusivity coefficient and the actual diffusivity value reduces as the concentration increases.

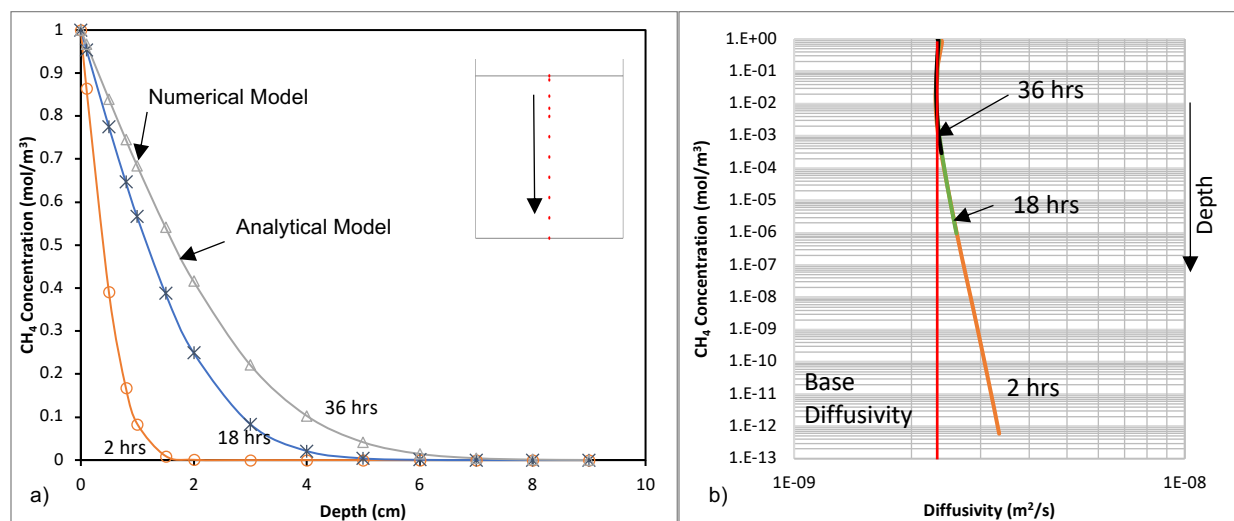


Figure 4 — a)  $\text{CH}_4$  concentration profile comparison between numerical and analytical models. b)  $\text{CH}_4$  concentration and diffusivity correlation as a function of depth in a log-log plot (Base diffusivity is the experimentally measured diffusivity).

In addition to validation using Dindoruk et al., the study by Teng et al. (2021) on the  $\text{CO}_2$ /brine system provided a visual representation of  $\text{CO}_2$  convective fingering through experiments. The simulation aligns well with the experimental results, accurately capturing the finger patterns at the same time steps and showing the evolution of finger thickness over time.

### Comparison between Experimental and Simulation Results

In this study, the effect of salinity is examined through four cases, as outlined in Table 2. The bulk diffusion coefficients used in the numerical modeling are derived from experimental measurements at varying salinities. The local grid refinement was found suitable for this investigation since it offers less numerical error. Figure 4a compares the pressure decay obtained from the experiment with the numerical simulation under Case 3 conditions. A notable discrepancy is observed at early times, indicating rapid dissolution. However, after four hours, the pressure in both the experiment and simulation aligns.

Table 2. Properties of the experimental cases

Cases	Temperature (°C)	Salinity (ppm)	Diffusion Coefficient (m <sup>2</sup> /s)
1	60	15	4.92
2	60	50	3.09
3	60	100	2.03
4	60	200	1.22

The CO<sub>2</sub> solubility in brine under Case 3 conditions was calculated using a tool (Dindoruk et al., 2023), yielding a value of 0.92 mol/kg, which corresponds to a maximum dissolved CO<sub>2</sub> mass of 31.8 g. Figure 4b illustrates the CO<sub>2</sub> mass dissolved and the development of convective fingers at three different stages: early time, the inflection point, and stabilized time. The maximum dissolved mass predicted by the numerical simulator aligns with the maximum dissolved mass computed based on the solubility for Case 3 conditions.

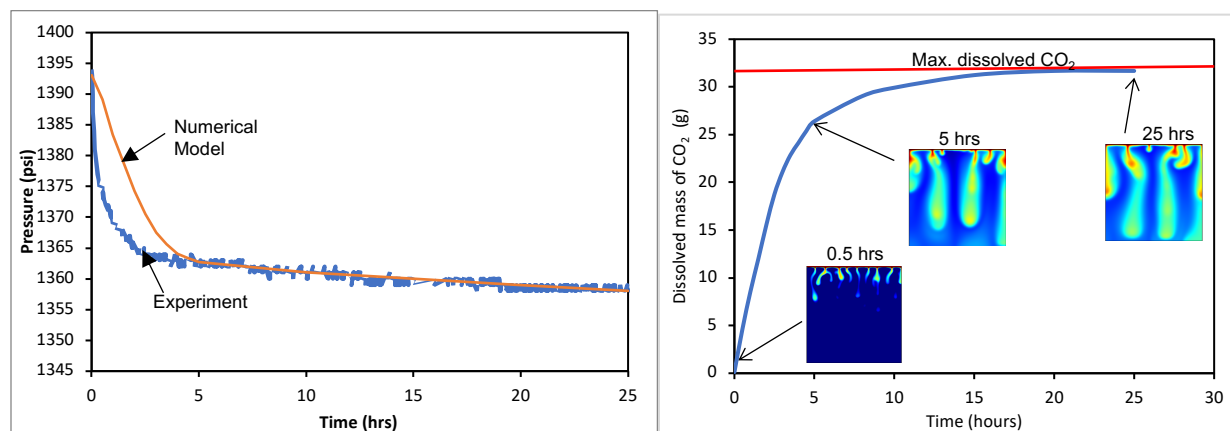


Figure 4 — a) Comparison between the experimental and numerical model pressure decay in the CO<sub>2</sub> domain, case 3. b) CO<sub>2</sub> dissolved mass profile and convective finger evolution for Case 3 at key time points.

## Conclusion

This study develops a robust numerical model to analyze CO<sub>2</sub> dissolution and convective mixing in brine, incorporating governing equations, boundary conditions, and experimental validation. Key findings highlight the importance of local grid refinement (LGR) for accurately capturing CO<sub>2</sub> fingering and minimizing numerical errors at the transition zone. Coarser grids, by contrast, overestimate CO<sub>2</sub> saturation and reduce symmetry in fingering patterns. The model exhibits strong agreement with experimental data for methane diffusion and CO<sub>2</sub> dissolution, supported by analytical back-calculations using Fick's second law, with deviations decreasing over time and higher concentrations.

Simulations successfully reproduce CO<sub>2</sub> convective finger morphology and evolution observed in experiments, emphasizing sensitivity to salinity, boundary conditions, and grid resolution. Higher salinity is shown to reduce CO<sub>2</sub> solubility and alter convective dynamics. The model aligns with experimental solubility data and pressure decay trends, validating its capability to simulate CO<sub>2</sub> dynamics in brine accurately. This tool offers critical insights for optimizing carbon sequestration strategies and predicting storage performance in saline aquifers. Future efforts should enhance diffusivity modeling at low concentrations and broaden experimental datasets for more comprehensive validation.

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