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Mechanistic Insights into Capillary Heterogeneity and Its Role in CO_2 Plume Confinement in Saline Aquifers

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Abstract

CO_2 storage in deep saline aquifers is governed by several trapping mechanisms, including structural, residual, solubility, and mineral trapping. Among these, residual trapping is regarded as one of the most secure long-term storage mechanisms; however, the relative contribution of local capillary trapping (LCT) versus pore-scale snap-off to the total residual inventory remains poorly quantified. LCT arises from strong spatial contrasts in capillary entry pressure between interbedded facies, particularly sand and shale, and can immobilize substantial volumes of CO_2 within the injection zone. In this study, LCT is quantified using a fully three-dimensional geostatistical reservoir model of interlayered sand–shale systems implemented in a compositional reservoir simulator. The results demonstrate that explicitly accounting for grid-block–scale capillary pressure heterogeneity increases the amount of locally trapped CO_2 by approximately 78% compared to a homogeneous capillary pressure representation. Sensitivity analyses were conducted to assess the effects of permeability variability in sand and shale facies, as well as reservoir inclination, on LCT. The findings indicate that increasing the coefficient of variation of sand permeability enhances LCT, whereas variations in shale permeability have a negligible effect. In contrast, increasing the reservoir inclination leads to a systematic reduction in LCT. A consistent inverse relationship is also observed between local capillary trapping and solubility trapping, with higher LCT corresponding to lower amounts of dissolved CO_2. Overall, the results underscore the importance of incorporating heterogeneous capillary pressure effects in reservoir-scale models to more accurately predict CO_2 trapping behavior and to ensure the long-term security of CO_2 storage in saline aquifers.

Introduction

Geologic carbon capture and storage has been identified as one of the most important ways by which the amount of anthropogenic CO_2 emissions in the atmosphere can be drastically reduced to achieve the net-zero carbon emissions target set by various countries [1,2]. Despite the immense benefits of geologic carbon storage, numerous issues hinder its widespread deployment. Key among the challenges is the issue of storage security. Thus, accurately accounting for each CO_2 trapping mechanism and its impact on CO_2 plume immobilization is critical. Of all the four CO_2 trapping mechanisms, residual trapping is the least well characterized. This is primarily because most CO_2 studies ignore the impact of local capillary trapping (LCT) [3]. Residual trapping can be divided into two categories: hysteresis/snap-off trapping and LCT. Hysteresis trapping is well understood, and most simulation studies focusing on CO_2 storage fully account for this residual trapping mechanism. Local capillary trapping, which results from wide spatial contrast in capillary pressure across facies, is, however, less well understood and is often ignored in simulation studies.

Earlier simulation studies by Saadatpoor et al. [4], focused on the impact of local capillary trapping during CO_2 storage, using the Leverett J function to scale the capillary pressure curve for each grid block. Gershenzon et al. [5] studied the effect of the Brooks-Corey (BC) and van Genuchten (VG) capillary pressure curve on the amount of LCT and dissolution trapping. The authors observed that the VG model underestimates the amount of LCT CO_2 and, consequently, the vertical migration of CO_2 within the plume. Ren and Jeong [6] further studied the impact of various flow regimes on the amount of LCT CO_2 in heterogeneous reservoirs. The results from the simulation study revealed that the amount of LCT CO_2 in viscous-dominated flow regimes is generally higher than that observed in buoyancy-dominated regimes. Ubillus et al. [7] also assessed the impact of the critical CO_2 saturation on the amount of LCT CO_2. The authors found that increasing the critical CO_2 saturation value leads to earlier onset of CO_2 local capillary trapping. Krishnamurthy et al. [8] also studied the impact of facies-scale differences on LCT CO_2 using surrogate fluids in a 2D beadpack experiment. The authors found that a low contrast between bead sizes led to an early breakthrough of CO_2, whereas the opposite effect was observed with a high contrast.

Despite the growing body of studies on local capillary trapping, many challenges remain unresolved. Firstly, most of the works on LCT have focused on 2D reservoirs, which do not accurately represent the actual flow of CO_2 in the subsurface. The injected $ScCO_2$ is physically prohibited from exhibiting radial dispersion which forces the fluid artificially to travel strictly in the lateral and vertical directions. This geometry profoundly distorts the true physical sweep efficiency of the plume. Because the fluid cannot spread radially to dissipate the pressure gradient and buoyancy forces, the rate of lateral advancement is artificially accelerated. Additionally, the impact of reservoir geologic parameters, such as the angle of inclination and the extent of permeability coefficient of variation, on LCT CO_2 in a 3D heterogeneous reservoir remains largely unexplored. This study addresses these gaps by evaluating the impact of geologic parameters, including inclination angle and coefficient of variation, on LCT magnitude in a highly heterogeneous 3D reservoir comprising sand and shale. Section 2 describes the theory and methods employed in this study. Section 3 presents the results and discussion of this study, while Section 4 provides concluding remarks.

Theory/Methods

The reservoir model for CO_2 sequestration was developed using the CMG-GEM compositional simulator (version 2025.10). An open-boundary system configuration was adopted to capture realistic flow and pressure dynamics, following the methodology of Wang et al. [9]. Open boundaries were implemented in CMG-GEM using the VOLMOD and TRANSI/TRANSJ/TRANSK keywords, which modify the effective volume and transmissibility of boundary cells, respectively. Boundary cells were assigned using a volume multiplier of 1000, while transmissibility was reduced by a factor of 0.1 to limit fluid exchange across the model boundaries. The injection well was located at the center of the reservoir model and perforated near the bottom at grid coordinates (I, J, K) = (25, 25, 163–165). Additional properties of the reservoir are presented in **Table 1**. Permeability values were assigned according to facies type. Sand facies were sampled from a log-normal distribution with a mean of 500 mD and a coefficient of variation (CV) of 0.6, while shale facies were sampled from a log-normal distribution with a mean of 0.01 mD and a CV of 0.5. Porosity values were generated using the empirical correlation proposed by Holtz et al. [10].

$$K_h = 7x10^7(\varphi^{9.61}) \tag{1}$$

Relative permeability and capillary pressure curves for both sand and shale facies were represented using the Brooks-Corey model. Further details on the relative permeability and capillary pressure curves can be found in [7] and [11] .
Capillary pressure was assigned on a grid-block basis using the Leverett J function (Eq. 2).

$$J(S_w) = \frac{P_C}{\sigma cos\theta}\sqrt{\frac{k}{\phi}} \tag{2}$$

Where $\sigma\ and\ \theta$ denote the interfacial tension and contact angle, respectively. It has been shown that reservoirs characterized by identical pore-size distributions share the same J function behavior [4]. This property enables the estimation of capillary pressure in individual grid blocks through scaling from a reference condition, under the assumption that wettability, which is largely controlled by interfacial tension and contact angle, does not vary spatially within the reservoir [12].

$$P_c(S_W) = P_{co}(S_W)\sqrt{\frac{\phi}{\phi_O}}\sqrt{\frac{k_o}{k}} \tag{3}$$

where $P_{co}, \phi_O\ and\ k_o$ represents the reference capillary pressure, porosity, and permeability, respectively.

Aquifer Properties	Values
Grid blocks	50 × 50 × 165
Permeability (mD) of sand	500
Permeability (mD) of shale	0.01
Reservoir temperature (°F)	142.5
Maximum bottom hole pressure (psi)	4500
Simulation Duration (years)	200
Injection Duration (years)	25
Depth at top (ft)	5,000
Injection rate (tons/day)	35

Table 1— Reservoir Parameters

Dimensional Numbers for CO₂ Plume Migration

In this study, we employed two-dimensional numbers to quantify the vertical and lateral movement of the CO_2 plume in the reservoir. In addition to the vertical center of mass, the aspect ratio was also employed.

The vertical center of mass of CO_2 in the z-direction is defined using the first spatial moment [11,13] :

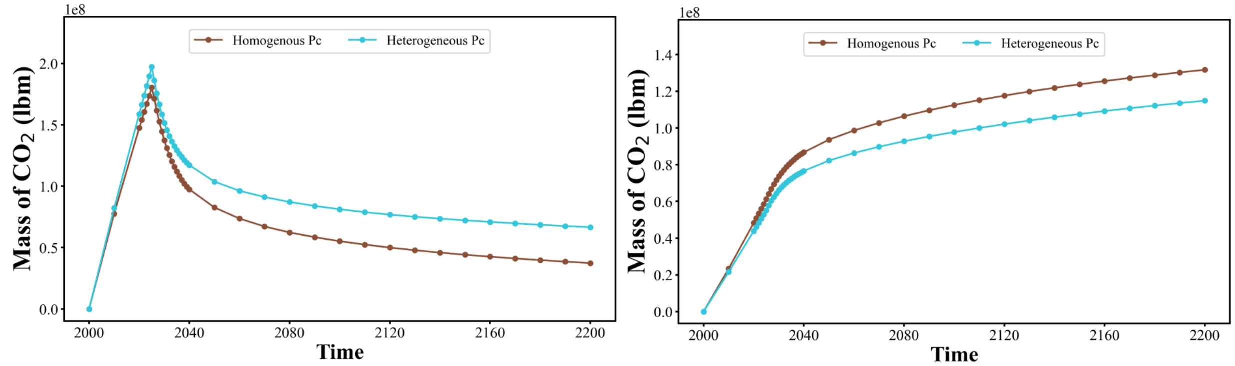
$$M_{i,j,k} = \int_0^{L_x}\int_0^{L_y}\int_0^{H} \emptyset(x,y,z)\,\rho(x,y,z)\,s(x,y,z)\,x^i y^j z^k\,dx\,dy\,dz \tag{4}$$

$$CM_z = \frac{M_{0,0,1}}{M_{0,0,0}} \tag{5}$$

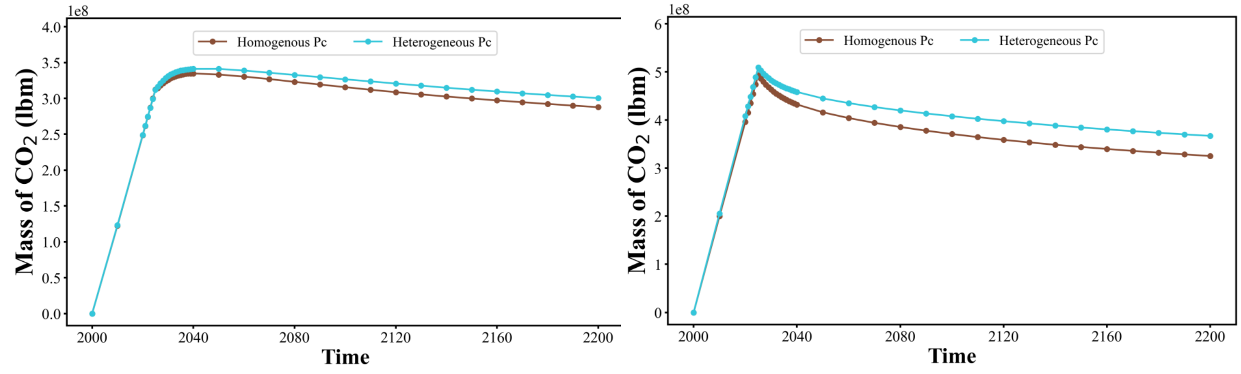
where CM_z is the vertical center of mass, $M_{0,0,0}$ is the zeroth moment (mass), $M_{0,0,1}$ is the first vertical moment (mass*length), ρ refer to the CO_2 density, s is the gas saturation, x, y, and z are the coordinates of each grid block. To further make this number dimensionless, we divided the value of CM by H (vertical thickness of the reservoir) to obtain a dimensionless number CM/H. The aspect ratio is defined as the ratio of the lateral to vertical movement of the CO_2 plume in the reservoir [7].

Results and Discussion

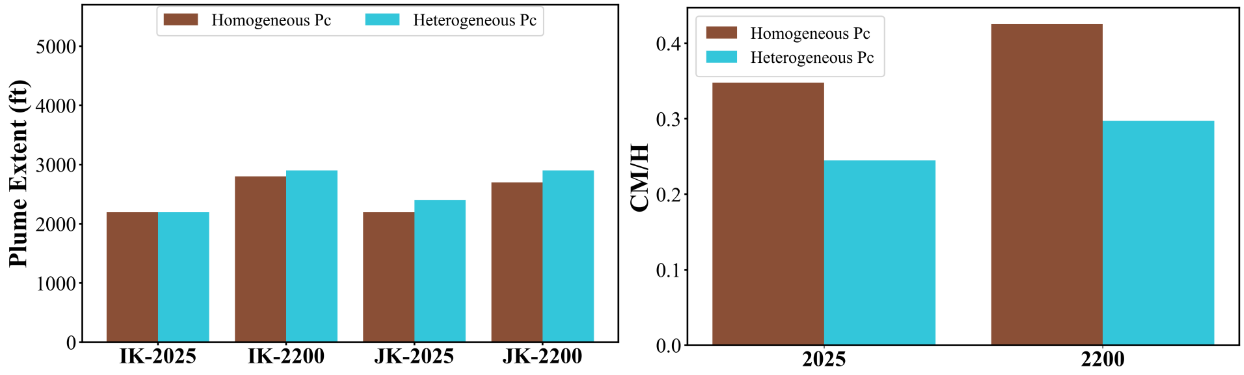
We initially evaluated the impact of homogeneous versus heterogeneous capillary pressure on the total amount of CO_2 stored through LCT. **Figure 1** presents the amount of CO_2 that is stored by the different trapping mechanisms for the two base cases (homogeneous and heterogeneous capillary pressure).



a. LCT **b. Dissolved CO_2**



c. Hysteresis **d. Total residual CO_2**



e. Horizontal CO_2 Movement **f. CM/H ratio**

Figure 1—Impact of Homogeneous and Heterogeneous capillary pressure on CO_2 trapping and plume migration over time

After 200 years, the heterogeneous capillary pressure scenario exhibits substantially greater local capillary trapping (LCT) of CO_2, with approximately 78% more CO_2 immobilized by LCT compared to the homogeneous capillary pressure case (**Figure 1a**). This enhanced trapping is accompanied by an inverse relationship between LCT and dissolution trapping. Specifically, the amount of dissolved CO_2 after 200 years is approximately 12.7% higher in the homogeneous capillary pressure model than in the heterogeneous capillary pressure model (**Figure 1b**). This behavior indicates that increased local capillary trapping reduces CO_2 availability for dissolution into the aqueous phase and vice versa.

These findings are further corroborated by the CO_2 plume migration patterns shown in **Figure 1 e-f**. Relative to the homogeneous capillary pressure model, the heterogeneous capillary pressure case displays a more pronounced lateral plume migration, with a 3.6% increase in plume extent in the IK direction and a 7.4% increase in the JK direction (**Figure 1e**). In contrast, vertical plume migration is more restricted, as reflected by the lower CM/H ratio observed in the heterogeneous case compared to the homogeneous case. The reduced vertical migration and enhanced lateral spreading observed in the heterogeneous capillary pressure model result from grid-block–scale variations in capillary pressure, which promote local capillary trapping and act as vertical flow barriers. By accounting for spatial variability in capillary pressure, buoyancy-driven upward migration of CO_2 is suppressed, forcing the plume to spread laterally and increasing residual trapping efficiency. This behavior is consistent with the physical mechanisms of local capillary trapping described in previous studies [12].

Sensitivity Analysis

We performed a sensitivity analysis to examine the impact of various factors, including the coefficient of variation of permeability in the sand and shale layers and the angle of inclination of the reservoir, on LCT CO_2 and plume migration. **Table 2** presents the parameters used for the base case.

Parameter	**Value**	**Unit**
Angle of Inclination	0	°
Coefficient of Variation (CV) of Sand	0.6	-
Coefficient of Variation (CV) of Shale	0.5	-

Table 2— Parameters for the Base Case

Impact of Shale and Sand Coefficient of Variation

Because the coefficient of variation (CV) plays a critical role in controlling permeability variability and reservoir heterogeneity, we investigated the influence of sand and shale CV on the amount of CO_2 immobilized through local capillary trapping (LCT). For the sand facies, two additional CV values (0.3 and 0.8) were evaluated alongside the base-case value of 0.6. Similarly, for the shale facies, two additional CV values (0.2 and 0.8) were considered in addition to the base-case value of 0.5.

For variations in the sand facies coefficient of variation (CV), the results show a strong dependence of local capillary trapping (LCT) on permeability heterogeneity. The case with a high sand CV of 0.8 exhibits significantly greater LCT than the cases with sand CV values of 0.3 and 0.5, with an approximately 70% and 375% increase observed between CV values of 0.3 and 0.8, for years 25 and 200, respectively, as shown in **Figure 2a**. This behavior reflects the role of increased sand permeability variability in enhancing reservoir heterogeneity, thereby promoting capillary barriers and increasing the effectiveness of LCT. However, we observed an inverse trend in dissolution trapping, with lower dissolution trapping at higher sand CV values (~23% and ~19% decrease between CV values of 0.3 and 0.8 at years 25 and 200, respectively). This observation is because increased heterogeneity reduces the extent of CO_2 convective mixing and, eventually, CO_2 dissolution. A similar observation was made by Tan et al. [14] in their study on the impact of layered heterogeneity on CO_2 convective reactive dissolution in saline aquifers.

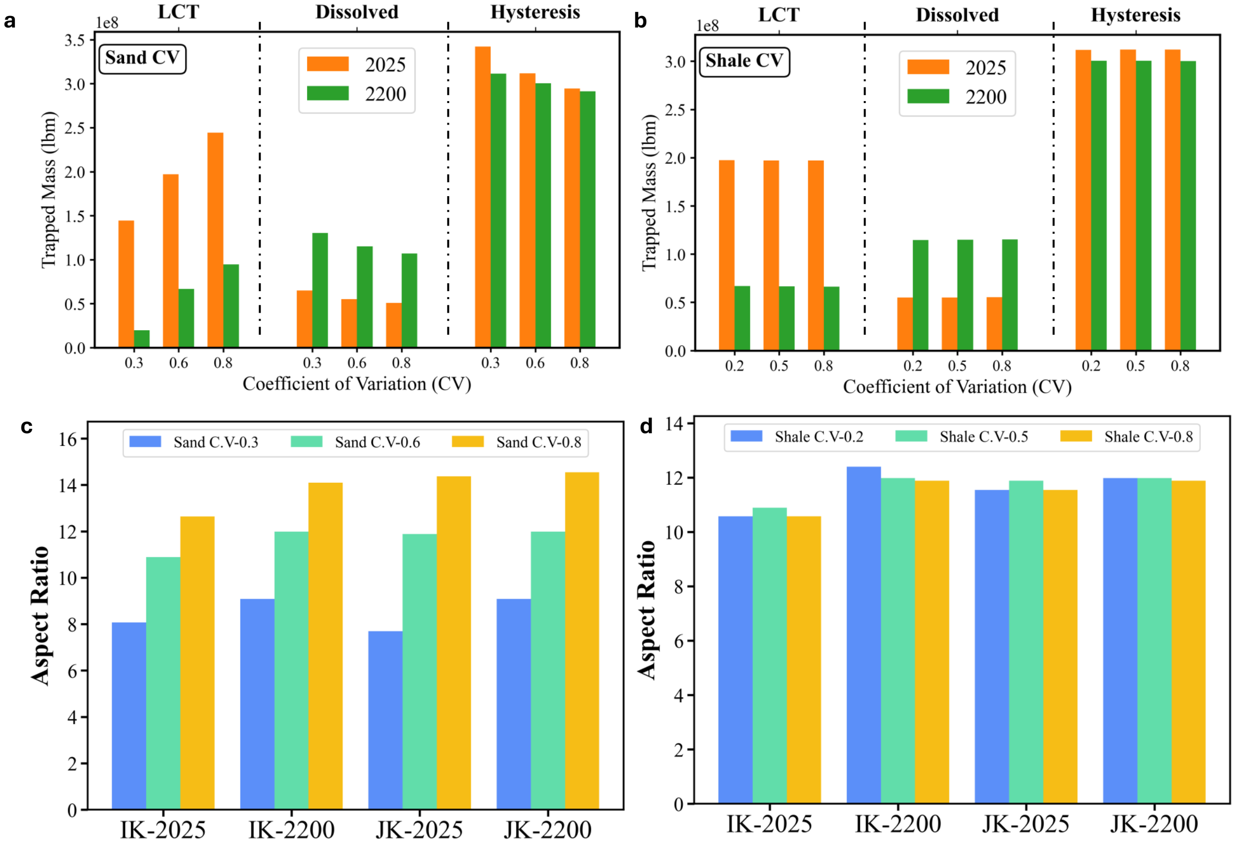
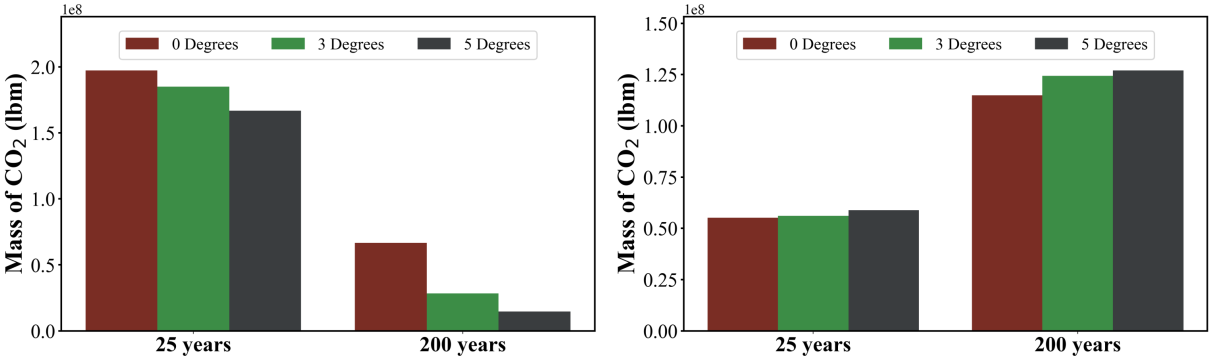


Figure 2—Impact of Sand (left) and Shale (right) Permeability Coefficient of Variation on CO_2 Trapping and Plume Migration

For variations in the shale facies coefficient of variation (CV), the impact on local capillary trapping (LCT) is negligible, with a difference of less than 1% observed across all cases. This limited sensitivity is attributed to the inherently low permeability of the shale layers (0.01 mD), such that changes in CV do not significantly alter the effective heterogeneity of the reservoir. This behavior contrasts with the sand facies, where the much higher mean permeability (500 mD) allows permeability variability to exert a stronger influence on flow and trapping processes. Similarly, variations in shale CV have a negligible effect on solubility trapping, with differences in dissolved CO_2 also remaining below 1% across all cases. This is because the shale has a significantly high capillary entry pressure making it an absolute barrier not contributing any flow paths for the injected CO_2. These findings are consistent with the CO_2 plume migration patterns shown in **Figure 2d**, which indicate no appreciable differences in plume aspect ratio among the shale CV scenarios.

Impact of Angle of Inclination

We further investigated the influence of reservoir inclination on local capillary trapping (LCT) and CO_2 plume migration. In addition to the base case with zero inclination, two inclined reservoir scenarios with dip angles of 3° and 5° were considered. The results show a pronounced reduction in LCT with increasing inclination angle. Relative to the horizontal case, the amount of locally trapped CO_2 decreased by approximately 57% and 78% for inclination angles of 3° and 5°, respectively. This observation is consistent with observations reported by Ren et al. [15] and reflects the enhanced buoyancy-driven flow along the dip direction, which limits the effectiveness of local capillary trapping. In contrast, dissolution trapping increases with reservoir inclination. After 200 years, the amount of dissolved CO_2 in the 5° inclination case is approximately 10.5% higher than that in the horizontal case, indicating that steeper inclination enhances CO_2–brine contact and promotes dissolution (**Figure 3**). Similar trends have been reported in previous studies by Chen et al. [16] and Callas et al. [17], further supporting the observed relationship between reservoir dip and CO_2 trapping.



a. LCT **b. Dissolved CO_2**

Figure 3—Impact of Angle of Inclination on CO_2 Trapping

Conclusions

In this study, we examined the impact of various reservoir parameters on LCT in a 3D reservoir consisting of interbedded sand and shale layers. The results from this study are summarized in Table 3:

Sensitivity Factor	Range Studied	Impact on LCT	Impact on Dissolution	Mechanistic Driver
Sand CV	0.3 to 0.8	+70% at year 25 +375% for year 200	-23% -19%	Increased frequency of flow barriers
Shale CV	0.2 to 0.8	Negligible (~1%)	Negligible	High Shale P_{ce} makes it an absolute flow barrier
Inclination	0° to 5°	-78%	10.50%	CO_2 bypasses local traps due to tilting

Table 3 —Summary of sensitivity analysis results and their mechanistic implications.

The results from the simulation lead to the following conclusions:

i. Incorporating heterogeneous capillary pressure drastically increased the amount of local capillary trapping in the reservoir. This was further supported by the enhanced lateral and suppressed vertical CO_2 plume migration in the heterogeneous capillary-pressure model compared to the homogeneous capillary-pressure model.
ii. Decreasing the angle of inclination led to a reduction in the amount of LCT CO_2.
iii. Increasing the sand coefficient of variation led to an increase in the amount of LCT CO_2, while varying the coefficient of variation of the shale layers had a negligible effect on the amount of LCT CO_2.
iv. In all the cases examined, we found a consistent inverse relationship between the amount of LCT CO_2 and dissolved CO_2.

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