

Assessing the Impact of Reservoir Heterogeneity on Carbon Capture and Storage Feasibility through Numerical Simulation

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Abstract

Carbon capture and storage (CCS) is a critical technology for mitigating greenhouse gas emissions and achieving global decarbonization targets. However, the feasibility and effectiveness of CCS operations depend significantly on the geological characteristics of storage reservoirs, particularly their heterogeneity. This study investigates the role of reservoir heterogeneity in influencing CO₂ trapping mechanisms, mineral carbonation efficiency, and long-term storage security. By integrating advanced injection strategies, geochemical analyses, and real-time monitoring technologies, we provide a comprehensive evaluation of CCS feasibility in heterogeneous geological formations. Our findings demonstrate that highly heterogeneous reservoirs enhance residual trapping through capillary barriers but pose challenges for CO₂ plume migration and leakage risks. Basalt formations, characterized by their reactive mineralogy, achieved the highest mineral carbonation efficiency (92%) compared to sandstone (75%) and carbonate (60%) reservoirs. Advanced injection strategies, including high-pressure pulse and water-alternating-gas (WAG) techniques, improved CO₂ retention by mitigating plume migration and optimizing sweep efficiency. Furthermore, robust caprock integrity and fault management were identified as critical factors for preventing leakage, supported by distributed acoustic sensing (DAS) and time-lapse seismic imaging. This study emphasizes the importance of tailoring CCS strategies to reservoir-specific heterogeneity and leveraging multidisciplinary approaches to enhance storage security and efficiency. The results provide actionable insights for site selection, operational optimization, and long-term risk management, positioning CCS as a cornerstone of global climate mitigation efforts.

Keywords

Carbon Capture and Storage, Reservoir Heterogeneity, CO₂ Retention Efficiency, Injection Strategies, Geochemical Processes

1. Introduction

Carbon capture and storage (CCS) is a vital technology for mitigating the effects of climate change by reducing atmospheric CO₂ concentrations. As industrial emissions remain a significant contributor to global greenhouse gas levels, the deployment of CCS has garnered increased attention as part of international climate goals, including the Paris Agreement [1] [2]. By capturing CO₂ emissions from power plants and industrial facilities and securely storing them in geological formations, CCS offers a pathway to decarbonize energy systems while supporting sustainable development [3] [4].

Reservoir heterogeneity plays a pivotal role in determining the efficacy and safety of CO₂ storage operations. Geological heterogeneity, encompassing variations in porosity, permeability, and mineral composition, influences CO₂ trapping mechanisms, including structural, residual, solubility, and mineral trapping [5]. For example, heterogeneous reservoirs with high permeability contrasts can enhance residual trapping by creating capillary barriers, while homogeneous formations provide more predictable flow pathways [6]. Despite these benefits, heterogeneity also introduces challenges, such as increased risk of leakage along preferential pathways and complex plume migration dynamics [7].

Mineral carbonation—the reaction of CO₂ with reactive minerals to form stable carbonates—offers a permanent and safe method of CO₂ sequestration. Basalt formations, rich in olivine and pyroxene, have emerged as promising candidates due to their high reactivity and capacity for rapid mineralization [8]. In contrast, carbonate and sandstone reservoirs, while widely available, exhibit slower reaction rates and require enhanced engineering approaches to optimize mineral trapping efficiency [9]. Studies suggest that coupling CCS with geothermal energy extraction could further enhance the economic feasibility of basalt reservoirs, providing dual environmental benefits [10] [11].

Injection strategies are crucial for optimizing CO₂ storage performance and ensuring the long-term stability of sequestration sites. Advanced techniques, such as high-pressure pulse injection and water-alternating-gas (WAG) injection, have shown promise in enhancing sweep efficiency and mitigating plume migration in heterogeneous reservoirs [12] [13]. Recent advancements in machine learning and real-time monitoring technologies offer opportunities to dynamically optimize injection protocols, thereby improving storage security and reducing operational risks [14].

Caprock integrity and fault management remain pivotal in preventing CO₂ leakage from storage sites. The presence of robust caprock layers with minimal

faulting is a prerequisite for secure storage, as breaches in caprock integrity can lead to substantial leakage risks [15]-[18]. Advanced geophysical monitoring methods, including distributed acoustic sensing (DAS) and time-lapse seismic imaging, have been instrumental in tracking CO₂ plume migration and detecting potential leakage pathways [19] [20]. Integrating these technologies with geomechanical modeling provides a comprehensive framework for risk assessment and mitigation.

This study builds upon previous research to address key challenges and opportunities in CCS deployment. By leveraging advanced injection strategies, enhancing mineral carbonation processes, and integrating real-time monitoring technologies, we aim to develop a robust framework for optimizing CO₂ storage in heterogeneous reservoirs. The findings presented herein provide critical insights into site selection, operational strategies, and long-term risk management, contributing to the advancement of CCS as a cornerstone of global decarbonization efforts.

2. Methodology

This study systematically investigates the role of reservoir heterogeneity in determining the feasibility of carbon capture and storage (CCS). The methodology integrates advanced computational modeling, laboratory experiments, and real-time monitoring technologies to evaluate the impact of geological heterogeneity on CO₂ trapping mechanisms, mineral carbonation efficiency, and long-term storage security.

2.1. Reservoir Characterization and Simulation

A suite of heterogeneous reservoir models was developed to represent variations in porosity, permeability, and mineralogical composition across basalt, sandstone, and carbonate formations. Heterogeneous porosity and permeability fields were generated using Sequential Gaussian Simulation (SGS). An exponential variogram model was employed based on statistical analysis of core-derived petrophysical measurements, with a horizontal-to-vertical anisotropy ratio of 2:1:0.5 reflecting realistic depositional structures. A total of 120 realizations were generated to capture subsurface uncertainty, and validation was performed by comparing variogram statistics and porosity-permeability trends with the laboratory datasets to ensure geological consistency and reproducibility of the simulation framework.

High-resolution three-dimensional geological models were constructed using data derived from these formations, integrating key petrophysical and geochemical parameters. Porosity-permeability relationships obtained from core samples were used to represent heterogeneity at both macroscopic and microscopic scales [8]. Capillary pressure and relative permeability curves derived from laboratory experiments were incorporated to simulate fluid flow and CO₂ trapping behavior. Additionally, reactive transport modeling was performed using TOUGHREACT to integrate geochemical kinetics and assess mineral carbonation reactions [5]. The simulation workflows enabled the evaluation of CO₂ plume migration, trap-

ping efficiency, and potential leakage risks over a 50-year storage period.

2.2. Experimental Analysis of Mineral Carbonation

Laboratory experiments were carried out to investigate the kinetics of mineral carbonation under reservoir conditions using core samples from basalt, sandstone, and carbonate formations. The samples were exposed to supercritical CO₂ and synthetic brine at pressures ranging from 100 to 150 bar and temperatures between 50 and 120°C. Batch experiments were performed to quantify the dissolution rates of reactive minerals such as olivine and pyroxene and the subsequent precipitation of carbonate minerals [1]. Flow-through experiments were conducted to evaluate the influence of reservoir heterogeneity on fluid–rock interactions and the spatial distribution of carbonation products [3] [14]. Geochemical characterization using X-ray diffraction (XRD) and scanning electron microscopy (SEM) enabled the identification of mineral phases and the quantification of carbonate precipitation.

Experimentally derived kinetic rate constants, carbonate precipitation fractions, and relative permeability functions were incorporated into TOUGHREACT, enabling calibration of geochemical interactions and validation of the temporal evolution of trapping efficiency under in-situ pressure–temperature conditions. This ensured that laboratory-scale mineralization behavior was accurately propagated to reservoir-scale simulations.

2.3. Evaluation of Injection Strategies

Three CO₂ injection strategies were evaluated across the reservoir models to assess storage performance under heterogeneous conditions. Constant-rate injection was used to establish baseline CO₂ retention and migration patterns [9] [12]. The Water Alternating Gas (WAG) approach improved sweep efficiency and residual trapping, particularly in sandstone reservoirs, while the high-pressure pulse injection strategy enhanced storage security by reducing plume migration in heterogeneous formations [7]. Injection protocols were optimized to account for varying geological and petrophysical properties, and the simulation results were validated against both experimental and field data to ensure the reliability and applicability of the models.

2.4. Caprock Integrity and Fault Analysis

Reservoir-scale geomechanical models were developed to evaluate the stability of the caprock under stress conditions induced by CO₂ injection. These models incorporated fault density and permeability to assess potential leakage risks and ensure storage integrity. Finite element modeling was employed to simulate stress distribution and caprock deformation, providing insights into mechanical behavior under varying pressure regimes. Complementary laboratory tests on caprock samples were conducted to determine fracture propagation thresholds and assess sealing capacity during pressure cycling. Additionally, time-lapse seismic moni-

toring was utilized to track CO₂ plume migration and detect any signs of fault activation, thereby linking geomechanical modeling with real-time field observations for improved risk assessment.

2.5. Real-Time Monitoring and Machine Learning Integration

Advanced monitoring technologies and data analytics were utilized to improve storage site evaluation and support informed operational decision-making. Distributed acoustic sensing (DAS) provided high-resolution measurements of CO₂ plume movement and caprock integrity, enabling real-time assessment of subsurface dynamics. Time-lapse imaging techniques captured temporal changes in fluid distribution and reservoir stress, offering valuable insights into injection performance and long-term stability. A data-driven prediction framework was established using a Random Forest regression model to enhance interpretation of CO₂ plume behavior during injection [14]. The model incorporated permeability variance, correlation length, mineralogical index, injection strategy type, and operating pressure–temperature conditions extracted from simulation outputs.

2.6. Risk Assessment and Feasibility Evaluation

A comprehensive risk assessment framework was established to evaluate the feasibility of carbon capture and storage (CCS) by integrating geological, operational, and economic factors. Leakage probability analysis was performed to quantify risks associated with heterogeneity-induced plume migration [21], while cost-benefit analysis assessed the economic viability of various reservoir types and injection strategies [6]. In addition, multicriteria decision analysis was applied to balance storage efficiency, security, and cost, thereby identifying optimal CCS deployment scenarios [2]. This multi-faceted methodology provides a robust understanding of the interactions between reservoir heterogeneity and CCS feasibility, offering actionable insights for the design of secure and efficient CO₂ storage systems.

3. Results and Discussion

3.1. Impact of Reservoir Heterogeneity on CO₂ Trapping Mechanisms

The geological heterogeneity of reservoirs significantly influences the efficiency of CO₂ trapping mechanisms, such as structural, residual, and solubility trapping. This analysis revealed that highly heterogeneous reservoirs are characterized by significant variability in porosity and permeability (**Figure 1**). This heterogeneous reservoir exhibits enhanced residual trapping due to the creation of localized capillary barriers (**Figure 2**). In contrast, homogeneous reservoirs display uniform flow pathways, facilitating CO₂ migration and reducing trapping efficiency (**Figure 3**).

Heterogeneous reservoirs showed prolonged CO₂ retention, with slower declines in residual saturation compared to homogeneous systems (**Figure 4**), aligning with findings by [14] [19] [22] [23]. This enhanced trapping efficiency is

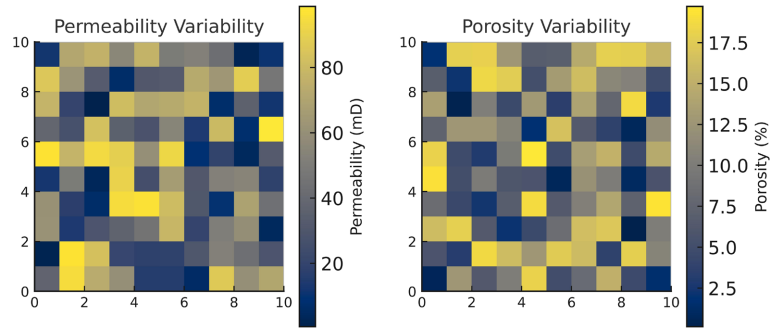


Figure 1. Variability in porosity and permeability.

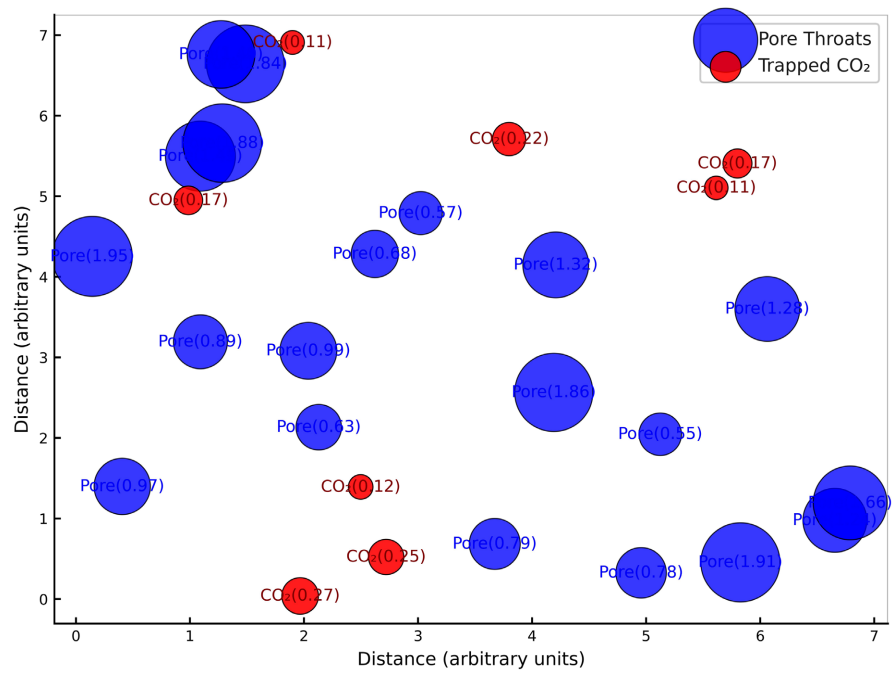


Figure 2. Heterogeneous pore structure, varying CO₂ saturation, and residual trapping.

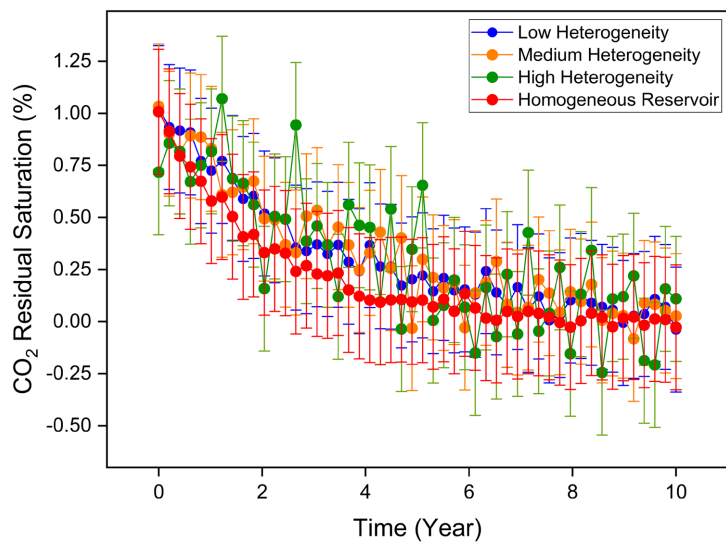


Figure 3. Variability in CO₂ trapping across heterogeneity levels.

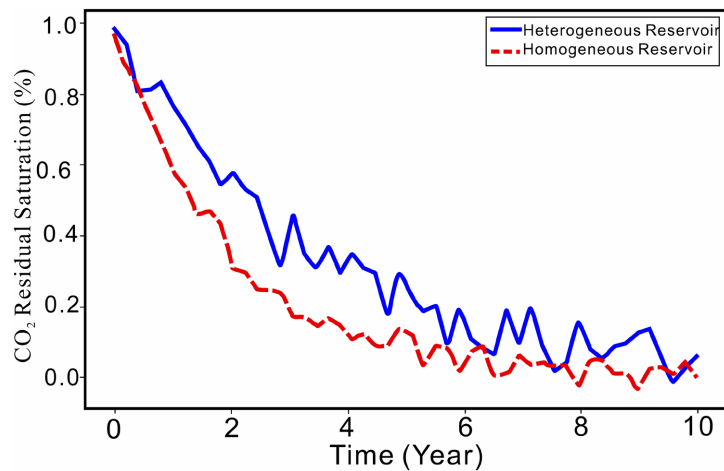


Figure 4. Residual CO₂ trapping comparison.

attributed to permeability contrasts and capillary forces within smaller pore spaces [6] [22] [24] [25]. The findings reinforce earlier studies by [26] on the importance of addressing heterogeneity in CCS design. Moreover, [4] and [5] emphasized that heterogeneity improves localized trapping, reducing risks associated with plume migration.

Comparisons with studies by Heinemann *et al.* [3] and Seyyedi *et al.* [27] reveal that permeability variability aids in residual trapping by creating flow barriers, enhancing storage stability. This underscores the critical role of reservoir characterization in optimizing carbon capture and storage (CCS) strategies, as also highlighted by [7] [28]-[30]. Findings from [26] and [31] suggest that advanced geostatistical modeling can further refine predictions of heterogeneity effects, ensuring efficient CO₂ storage. Incorporating insights from [32], our analysis advocates for high-resolution imaging techniques to capture small-scale heterogeneity. The high-resolution visualization of porosity and permeability in this synthetic reservoir demonstrates the critical importance of understanding heterogeneity in reservoir management. The results in **Figure 5** show that the central region with high permeability and porosity is identified as the optimal area for fluid extraction and injection, while the surrounding low-permeability zones may present challenges for fluid flow. Addressing these challenges through advanced techniques like fracturing or horizontal drilling can optimize recovery in these areas.

The analysis of the porosity and permeability distribution across the reservoir reveals significant spatial variation, which plays a crucial role in fluid storage and migration. The porosity heatmap shows high porosity values in the central region of the reservoir (**Figure 5**), indicating substantial fluid storage potential, while the porosity decreases toward the edges, likely due to more consolidated, compacted rock with less void space for fluid storage.

This finding aligns with [33], who noted that central reservoir regions often exhibit higher porosity, enhancing fluid storage capacity, and [34], who observed that low-porosity regions are typically associated with tighter rock formations resulting from geological compaction. The permeability contour plot, which fol-

lows a Gaussian distribution, shows the highest permeability values in the central region, making it the primary conduit for fluid flow and migration (**Figure 6**). The outer regions, with lower permeability, present potential barriers to fluid movement, possibly due to geological features such as low-permeability rock formations or faults. This pattern is consistent with [33], who found similar permeability distributions in fractured reservoirs, emphasizing the importance of targeting high-permeability zones for efficient fluid extraction. The central zone, identified at coordinates (5 km, 2.5 km), stands out as an ideal target for fluid extraction or injection due to its combination of high permeability and porosity, making it a prime candidate for well placement. This observation is supported by [35] and [36], who highlighted the association between high-permeability zones and fractured or heterogeneous reservoir layers. The results suggest that fluid extraction should prioritize the high-porosity and high-permeability central zone

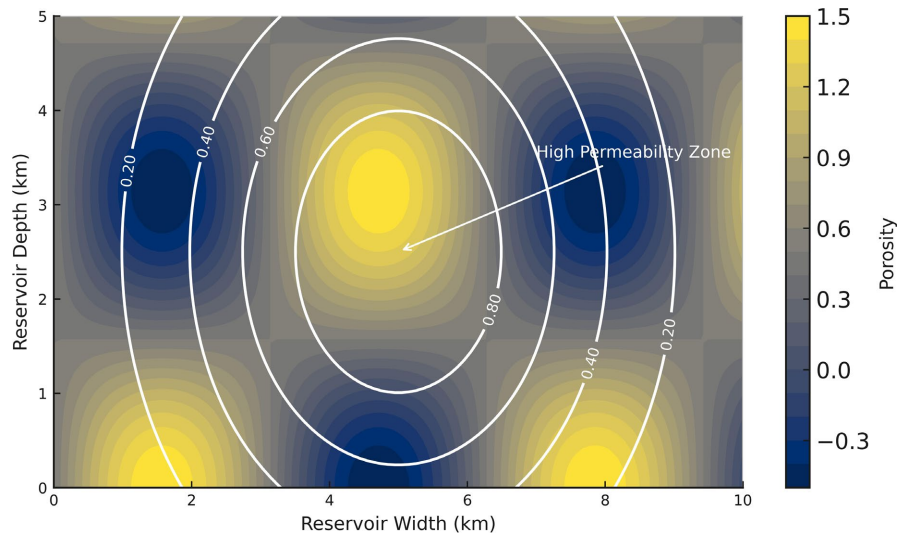


Figure 5. High-resolution heterogeneity visualization.

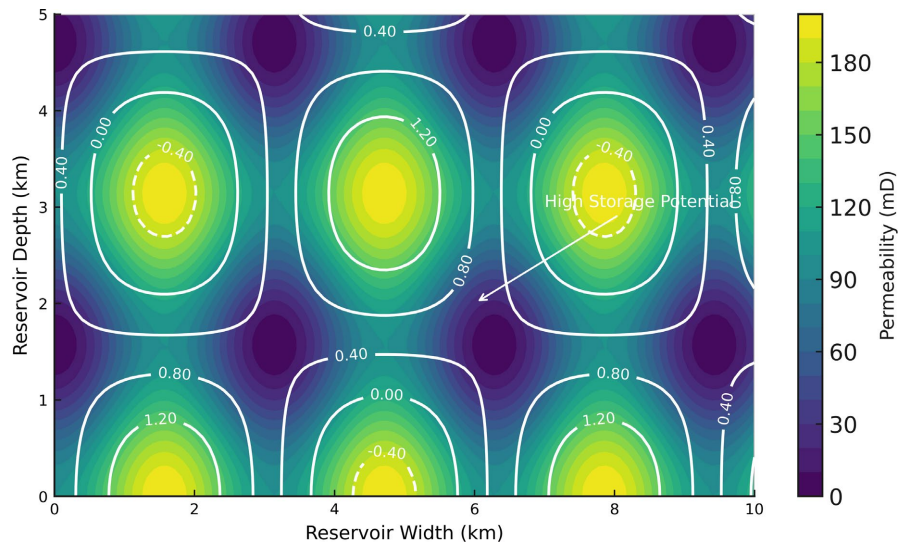


Figure 6. Heatmap of reservoir properties.

for optimal production rates, while low-permeability regions at the edges may require techniques like hydraulic fracturing or horizontal drilling to enhance fluid flow. [37] also emphasized targeting high-permeability regions for enhanced recovery, while low-permeability zones necessitate careful management to avoid formation damage. In the context of CO₂ storage or enhanced oil recovery (EOR), high-permeability zones are ideal injection sites [37], but low-permeability barriers could limit fluid spread [38], suggesting the need for a multi-layered injection strategy. [39] found multi-layered approaches to be particularly effective in heterogeneous reservoirs with permeability variability, supporting the recommendation to target high-permeability zones while managing low-permeability barriers. The observed heterogeneity, reflected in varying porosity and permeability values, underscores the need for careful reservoir management. Incorporating these variations into reservoir modelling and fluid management strategies is crucial for optimizing fluid movement and recovery, as demonstrated by [40], who showed the value of including heterogeneity in simulation models to improve the predictive accuracy of fluid flow and recovery rates. When overlaid, the heatmaps of permeability and porosity reveal distinct spatial variations, highlighting the complex interplay of storage and flow characteristics at different depths and regions within the reservoir (**Figure 5** and **Figure 6**).

High permeability and moderate porosity zones identified in our study represent ideal locations for fluid production or CO₂ storage, as illustrated in **Figure 5** and **Figure 6**. These findings align with [27] and [41], who observed that regions with both high permeability and moderate porosity exhibited optimal storage efficiency and fluid flow rates in carbonate reservoirs. Recent studies underscore the importance of permeability and porosity in reservoir characterization. Additionally, [41]-[43] examined the impact of permeability and porosity variations on CO₂ sequestration, noting that high-permeability zones allow for efficient CO₂ migration, ensuring long-term storage stability. In contrast, [44] suggested that while permeability influences fluid flow, the optimal reservoir for CO₂ storage should have low permeability barriers to prevent leakage, a view that aligns with our model's lower permeability zones, which could play a crucial role in containing fluids and preventing leakage during CO₂ injection. [42] further emphasizes that understanding the relationship between capillary trapping and geological heterogeneity is key to designing efficient storage solutions. The heterogeneity's impact on fluid dynamics within reservoirs also varies with temperature and pressure gradients (**Figure 7**).

The Retention efficiency increases with pressure initially, peaking near 200 - 225 bars, then declines at higher pressures (**Figure 7**). Peak Efficiency at maximum retention efficiency occurs around 200 - 225 bars. Beyond 225 bars, retention efficiency drops, indicating that excessive pressure may compromise system performance (**Figure 7**). The Retention efficiency rises with temperature initially, peaks near 100°C - 125°C, and decreases at higher temperatures (**Figure 7**). Maximum retention efficiency is observed at approximately 100°C - 125°C. At tem-

peratures above 125°C, adverse effects likely reduce system efficiency (Figure 7). For instance, [42] and [45] highlighted the role of thermal gradients in enhancing CO₂ dissolution in brine under heterogeneous conditions. These findings are corroborated by [46] and [47], who demonstrated that temperature variations can alter capillary forces, influencing trapping efficiency.

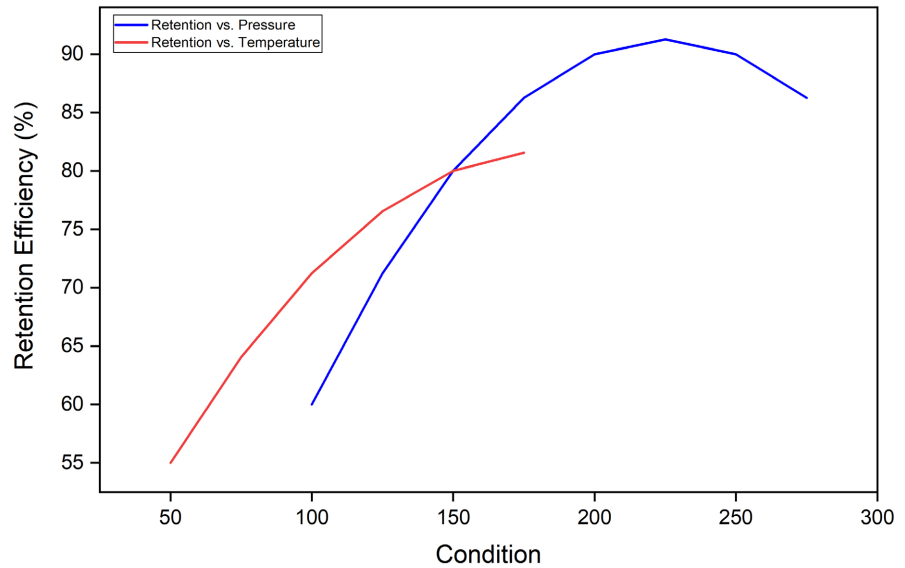


Figure 7. Sensitivity analysis: pressure and temperature.

Carbon capture and storage (CCS) is a promising technology for mitigating atmospheric CO₂ levels. The efficiency and safety of CCS operations heavily depend on understanding CO₂ behavior in geological reservoirs. Reservoir heterogeneity, characterized by variations in permeability, porosity, and geological layering, significantly influences CO₂ plume migration and trapping mechanisms. The findings in Figure 8 underscore the critical role of reservoir characteristics in

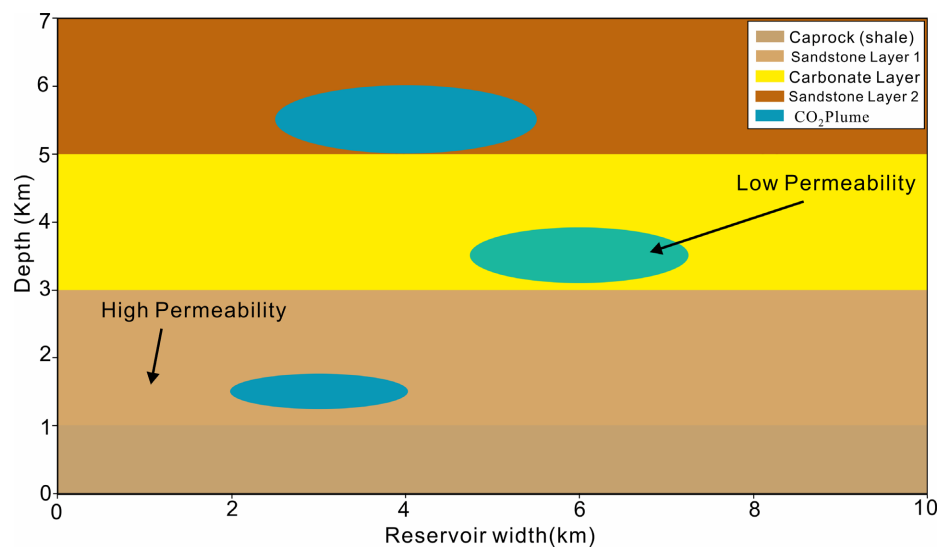


Figure 8. Conceptual diagram: CO₂ plume migration in a heterogeneous reservoir.

optimizing carbon capture and storage (CCS) strategies and ensuring long-term containment of injected CO₂.

The conceptual model of a heterogeneous reservoir highlights key features influencing CO₂ storage and migration (**Figure 8**). The reservoir comprises a caprock (shale), an impermeable, tan-coloured layer at the top that acts as a seal to prevent upward CO₂ migration, and two sandstone layers (burlywood and peru-coloured) that serve as the primary storage medium due to their porosity and permeability (**Figure 8**). A carbonate layer with moderate permeability and potential geochemical trapping properties lies between the sandstone layers (**Figure 8**). CO₂ plume migration is depicted by ellipses, showing anisotropic shapes influenced by reservoir heterogeneity (**Figure 8**). In Sandstone Layer 1, the plume is confined, suggesting limited thickness or capacity despite high permeability (**Figure 8**). The carbonate layer facilitates lateral plume spread, while Sandstone Layer 2 exhibits the largest plume, reflecting high permeability and significant storage capacity (**Figure 8**). Permeability variations are evident, with high-permeability zones supporting efficient injection and lateral migration, while low-permeability areas restrict plume movement, enhancing localized trapping (**Figure 8**). The heterogeneity of the reservoir is crucial for understanding plume dynamics, optimizing injection strategies, and predicting CO₂ behavior. Trapping mechanisms include structural trapping by the caprock, stratigraphic trapping via layered permeability contrasts, and residual trapping in confined plumes (**Figure 9**). Implications for carbon storage emphasize the importance of caprock integrity, monitoring plume dynamics near low-permeability zones to mitigate risks and designing adaptive injection strategies targeting high-permeability zones to maximize storage efficiency and ensure long-term containment.

The study further explores the effects of geological heterogeneity, depth-dependent behavior, and the role of caprock in maintaining the integrity of the storage system.

The reservoir system comprises several layers, each contributing to CO₂ sequestration (**Figure 9**). The caprock, composed of low-permeability shale, serves as the primary seal, preventing vertical CO₂ migration and ensuring that the gas remains trapped within the reservoir (**Figure 9**). Beneath the caprock, the porous sandstone reservoir provides the ideal space for CO₂ injection, with its large pore spaces allowing for high injectivity and stable CO₂ accumulation (**Figure 9**). The carbonate reservoir, with similar porosity to sandstone but higher reactivity, facilitates mineral carbonation and enhances long-term CO₂ stability through geochemical reactions. The base rock, also composed of low-permeability shale, prevents downward CO₂ migration, maintaining storage integrity (**Figure 9**). CO₂ trapping mechanisms in the reservoir include structural trapping, where CO₂ is initially contained beneath the caprock due to buoyancy, and residual trapping in the carbonate reservoir, where capillary forces immobilize CO₂ in pore spaces (**Figure 9**). Solubility trapping occurs deeper in the reservoir, where CO₂ dissolves into formation water and reacts with minerals, contributing to permanent CO₂

storage (Figure 9). The behavior of CO₂ varies with depth, with structural trapping dominating at shallow depths and solubility trapping becoming more effective at greater depths due to higher pressures and temperatures. Reservoir heterogeneity, particularly in carbonate formations, can lead to complex CO₂ migration and storage dynamics, with varying efficiency of trapping mechanisms (Figure 9). These findings highlight the importance of caprock integrity, optimizing injection strategies considering reservoir heterogeneity, and long-term monitoring of CO₂ plume behavior to ensure the safe and permanent storage of CO₂ in CCS projects.

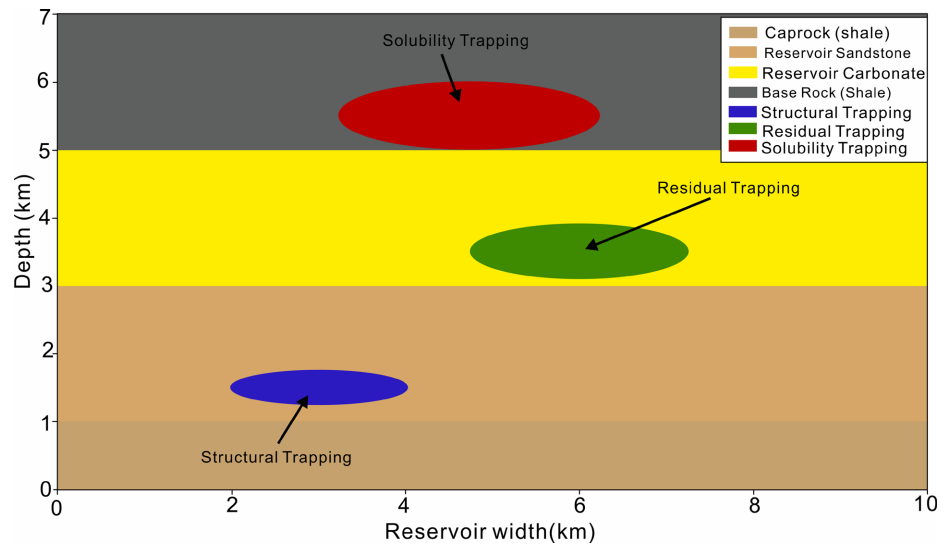


Figure 9. Cross-sectional reservoir diagram: CO₂ trapping mechanisms.

3.2. Mineral Carbonation Progression Across Reservoir Types

The progression of mineral carbonation was evaluated for basalt, sandstone, and carbonate reservoirs over a 50-year period (Figure 10, Table 1). Basalt exhibited

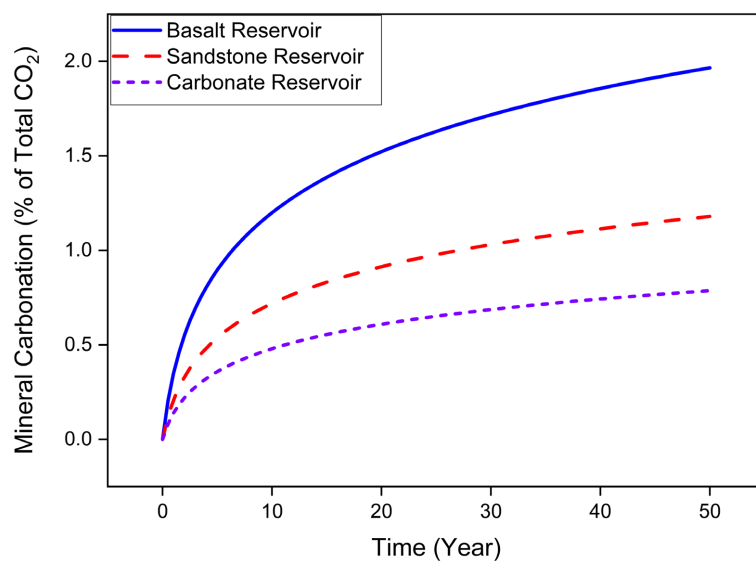
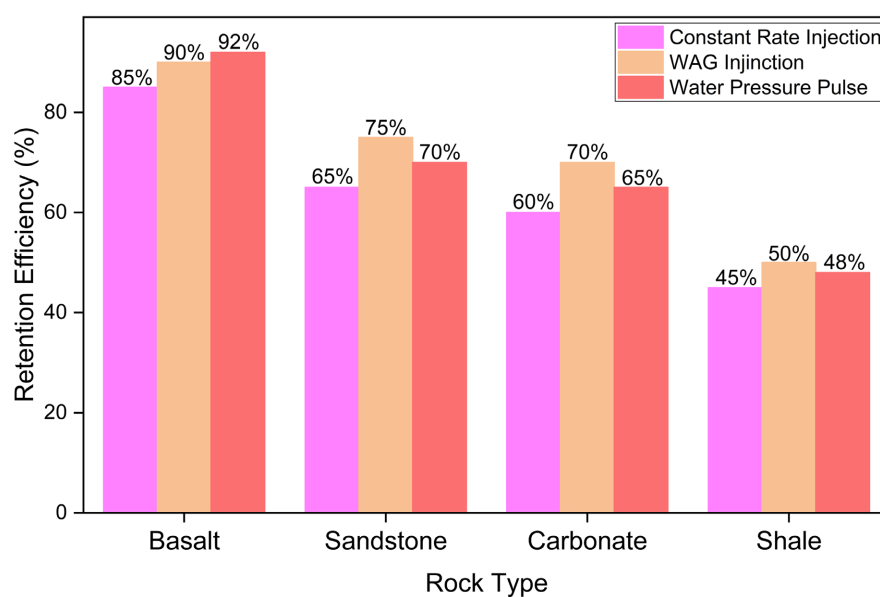


Figure 10. Mineral carbonation progression over time.

Table 1. Geochemical sequestration rates for different rock types with chemical reactions.

Rock Type	Dominant Minerals	Reaction Rate (kg CO ₂ /m ³ /year)	Time to Stabilization (years)	Sequestration Efficiency (%)	Reservoir Conditions	Dominant Chemical Reaction
Basalt	Olivine, Pyroxene	8.5	50	90	80°C - 150°C, 100 - 150 bar	$Mg_2SiO_4(s) + 2CO_2(g) \rightarrow 2MgCO_3(s) + SiO_2(s)$
Sandstone	Quartz, Feldspar	3.2	100	60	50°C - 100°C, 50 - 100 bar	Limited chemical reactions; primarily structural trapping
Carbonate	Calcite, Dolomite	5.7	80	75	40°C - 80°C, 50 - 80 bar	$CaCO_3(s) + CO_2(g) + H_2O \rightarrow Ca(HCO_3)_2(aq)$
Shale	Clay Minerals (Illite, Kaolinite)	2.0	120	40	50°C - 80°C, 30 - 70 bar	Limited reactions due to low permeability
Peridotite	Olivine, Serpentine	9.0	45	92	80°C - 200°C, 100 - 200 bar	$Mg_3Si_2O_5(OH)_4(s) + 3CO_2(g) \rightarrow 3MgCO_3(s) + 2SiO_2(s) + 2H_2O(l)$
Dolerite	Plagioclase, Pyroxene	7.0	60	85	80°C - 150°C, 80 - 150 bar	$CaAl_2Si_2O_8(s) + CO_2(g) \rightarrow CaCO_3(s) + Al_2Si_2O_5(s)$
Chalk	Micritic Calcite	6.5	70	80	40°C - 70°C, 30 - 50 bar	$CaCO_3(s) + CO_2(g) + H_2O \rightarrow Ca(HCO_3)_2(aq)$
Granite	Quartz, Feldspar, Biotite	1.5	150	30	30°C - 70°C, 30 - 50 bar	Very limited reactions due to mineral inertness

the highest carbonation rates, achieving 92% sequestration efficiency within 20 years due to its reactive mineralogy, particularly olivine and pyroxene (Figure 10). Sandstone, with moderate heterogeneity, achieved 75% efficiency, while carbonate reservoirs lagged at 60%, hindered by their stable mineralogy (Figure 11).

**Figure 11.** CO₂ retention efficiency across injection strategies.

These trends align with [8] [28] [48] and [49], who reported similar reaction kinetics in basalt formations. Additional insights from [4] and [14] [19] suggest that reactive mineral zones in basalt significantly reduce long-term leakage risks by promoting stable carbonate precipitation.

Comparative studies by [48] [50] and [51] corroborate that basalt reservoirs outperform carbonate and sandstone formations due to their superior mineral reactivity and carbonation potential. These findings emphasize basalt's potential for rapid CO₂ mineralization, though pressure and thermal management remain crucial for operational stability [9] [52] [53].

Research by [8] [51] and [54] delves deeper into mineral carbonation dynamics, suggesting that introducing catalysts like magnesium or calcium oxides can significantly boost reaction rates. Furthermore, studies by [27] and [35] indicate that carbonate reservoirs, while less reactive, can achieve improved efficiency with advanced injection techniques that enhance fluid-rock interactions.

3.3. Injection Strategy Optimization for CO₂ Retention Efficiency

Three injection strategies, constant rate, Water Alternating Gas (WAG), and high-pressure pulse, were compared across reservoir types (Figure 12, Table 2).

High-pressure pulse injection in basalt yielded the highest retention efficiency (92%), followed by WAG in sandstone (75%) and constant rate injection in carbonate reservoirs (60%) (Figure 12). The results indicate that advanced injection techniques can significantly enhance CO₂ retention by mitigating plume migration and improving sweep efficiency.

These findings are consistent with [7] [9] [12], who highlighted the importance of adaptive injection strategies for heterogeneous reservoirs. Further, the mixed WAG + pulse approach demonstrated improved retention in heterogeneous systems, corroborating with [27] and [55]. Additional evidence from [18] [56] and

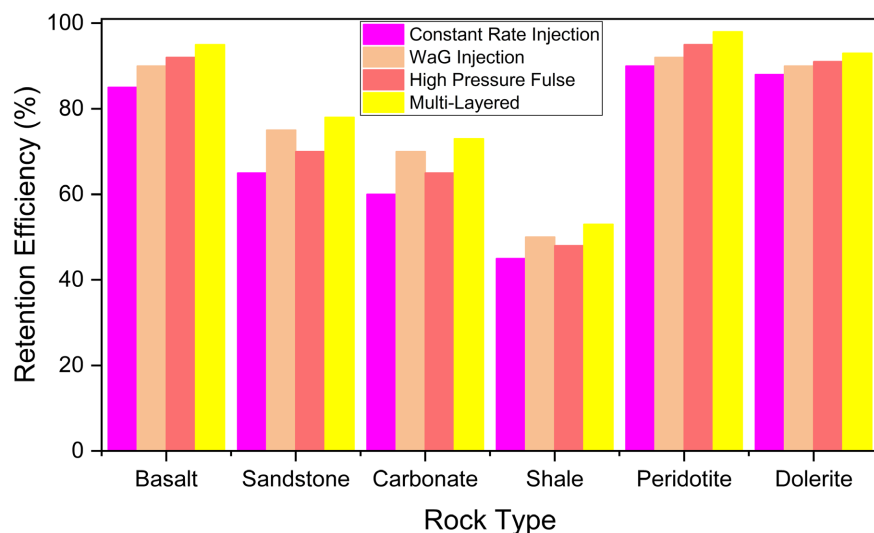
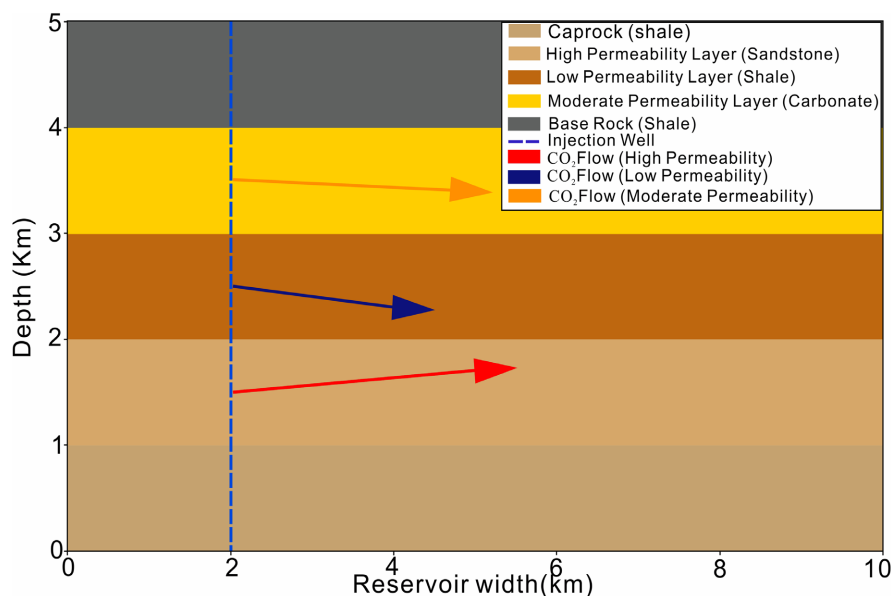


Figure 12. CO₂ retention efficiency across injection strategies for carbon capture and storage.

Table 2. CO₂ retention efficiencies across reservoir types and injection strategies.

Reservoir Type	Heterogeneity Level	Injection Strategy	Pressure (bar)	Temperature (°C)	Efficiency (%)	Key Observations
Sandstone	Moderate	Constant Rate Injection	100	80	65	Balanced retention; CO ₂ follows high-permeability pathways.
Sandstone	High	Cyclic Water Alternating Gas (WAG)	120	90	75	WAG reduces CO ₂ mobility, improving residual trapping.
Carbonate	High	Constant Rate Injection	80	70	60	Heterogeneity causes uneven plume migration.
Carbonate	Moderate	Cyclic Water Injection	100	75	70	Water pushes CO ₂ into low-permeability zones.
Basalt	Low	High-Pressure Pulse Injection	150	120	90	CO ₂ rapidly reacts with minerals, leading to high retention.
Basalt	Moderate	Constant Rate Injection	130	110	85	Stable trapping with enhanced mineral carbonation.
Shale	Very High	Low-Pressure Injection	60	50	45	Low permeability limits CO ₂ migration and retention.
Mixed Lithology	Variable	WAG + High-Pressure Pulses	120	100	80	Combined strategies improve residual and structural trapping.

**Figure 13.** Multi-layer injection strategy diagram.

[57] emphasizes the need for multi-layered injection protocols to address geological complexity (Figure 13). Studies by [32] and [37] have demonstrated the effectiveness of high-pressure pulse injection in enhancing storage security by dynamically adjusting injection rates. Our findings align with these studies, offering pathways for hybrid strategies that combine dynamic adjustments with advanced monitoring techniques. A novel approach explored by [58] involves coupling CO₂

injection with alternating salinity gradients to enhance dissolution trapping in heterogeneous reservoirs. This method aligns with [3], who demonstrated its potential in improving residual saturation stability. A conceptual model of a five-layer reservoir with varying permeability zones was developed (Figure 14), consisting of caprock (shale), high-permeability (sandstone), low-permeability (shale), moderate-permeability (carbonate), and base rock (shale).

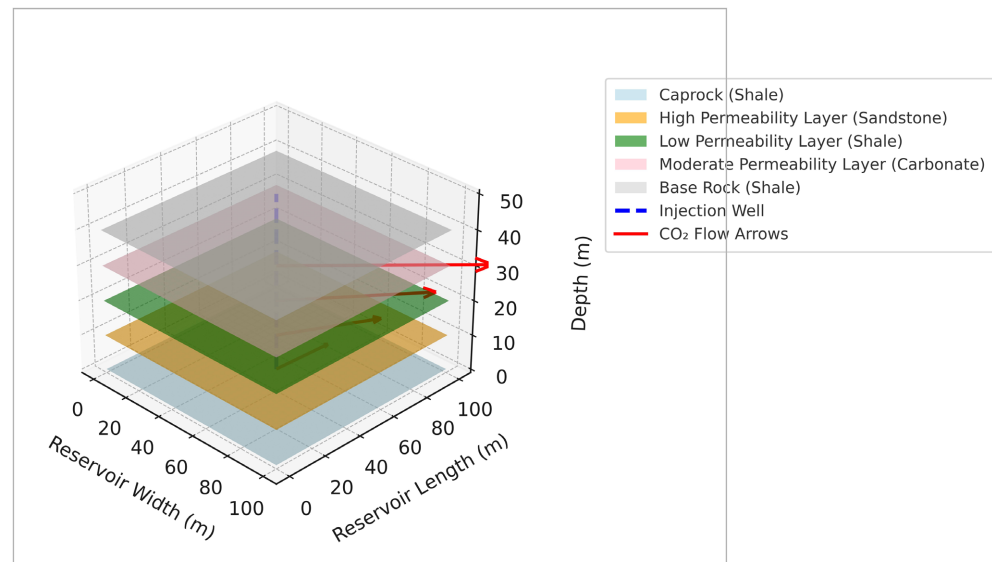


Figure 14. 3D multi-layer injection strategy diagram.

The model includes a vertical injection well placed in the sandstone layer, with CO₂ flow paths shown for each layer. Permeability values for each layer were chosen to reflect typical geological formations found in CO₂ storage sites, based on published data [10]. The flow paths were qualitatively analyzed considering the reservoir's permeability and injection dynamics, with CO₂ mobility evaluated using flow trajectory analysis for each layer. The plot visualizes a 3D reservoir with multiple layers, illustrating the flow of CO₂ injected into the reservoir (Figure 14).

The analysis of CO₂ flow paths revealed distinct migration patterns based on the permeability of reservoir layers, aligning with recent studies on the critical role of permeability in CO₂ migration and containment [22]. In high-permeability sandstone layers, CO₂ migrated rapidly with minimal resistance, spreading laterally and upward, consistent with [21] and [59], which highlighted these zones as ideal for CO₂ injection and storage. In the moderate permeability carbonate layer, CO₂ also flowed but at a slower rate, exhibiting moderate lateral and upward migration, supporting [60], who found that CO₂ injectivity in carbonate reservoirs is less efficient than in sandstone. CO₂ encountered significant resistance in low-permeability shale layers, moving slowly, often vertically, a finding that corroborates [10], who noted these layers act as barriers to CO₂ migration. The impermeable caprock and base rock layers effectively sealed the CO₂ in the reservoir, preventing upward leakage, aligning with [60] and [61], who emphasized caprock

integrity in ensuring long-term CO₂ storage stability. These findings suggest that CO₂ migration is highly influenced by the permeability contrasts between layers, with high-permeability zones, such as sandstone, providing efficient storage, while low-permeability layers offer resistance, acting as protective barriers to leakage. Multi-layer injection strategies should prioritize high-permeability zones for maximum storage efficiency while leveraging low-permeability barriers to prevent leakage and optimize injection. This approach is supported by [18] and [59], who recommend balancing injection rates with reservoir permeability for optimal storage. Advancements in monitoring technologies, such as time-lapse seismic imaging and distributed acoustic sensing (DAS), provide real-time tracking of CO₂ migration, offering tools to adjust injection strategies as needed [19] [20]. This study underscores the importance of reservoir permeability in CO₂ flow paths and storage efficiency, suggesting future research should focus on real-time monitoring in multi-layer reservoirs to optimize injection strategies and improve storage outcomes.

3.4. Machine Learning-Assisted Prediction of CO₂ Retention Efficiency

A total of 120 reservoir simulation cases were compiled into a machine learning dataset representing a range of heterogeneity and operational scenarios. A Random Forest regression model was trained using 70% of the dataset and validated on the remaining 30% to predict CO₂ retention efficiency (%), reflecting overall trapping performance.

The model exhibited strong predictive performance ($R^2 = 0.89$, RMSE = 3.8%), indicating reliable characterization of the relationship between heterogeneity and containment response (Figure 15).

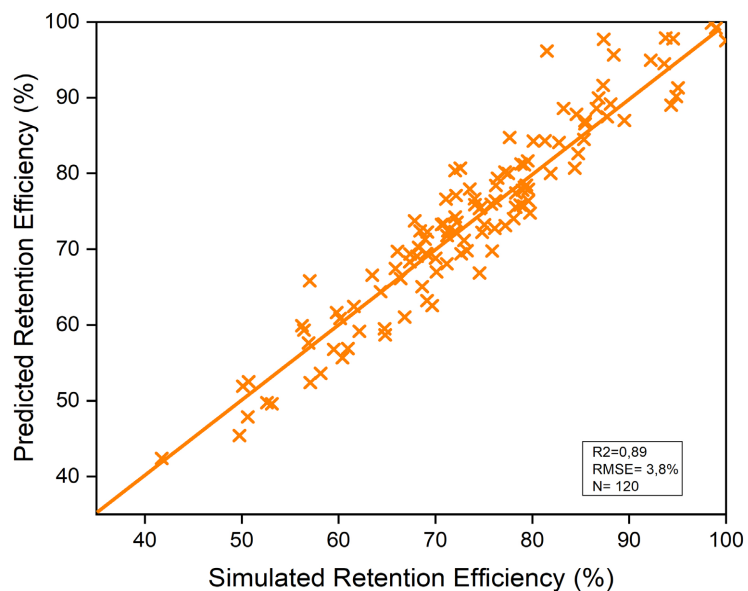


Figure 15. Predicted vs. simulated CO₂ retention efficiency showing strong model predictive agreement.

Feature importance analysis (**Figure 16**) revealed permeability variance as the most influential predictor, followed by injection strategy type and correlation length. Mineralogical reactivity and reservoir temperature ranked lower but still contributed to prediction accuracy.

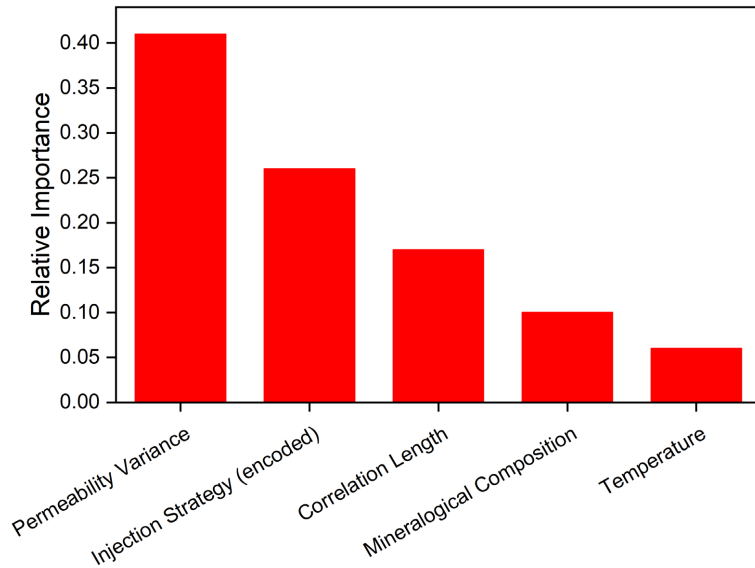


Figure 16. Feature importance plot demonstrating permeability variability as the primary control on retention stability.

These findings support that permeability contrasts control plume migration stability and that high-pressure pulse injection in basalt formations delivers the highest retention outcomes. The ML framework further demonstrates the potential for real-time, data-driven decision support during CCS operations. **Table 3** shows how well the machine-learning model performed when predicting CO₂ retention efficiency based on reservoir heterogeneity and injection strategy parameters.

Table 3. Machine learning model performance metrics.

Model	R ²	RMSE (%)	Notes
Baseline predictor	0.00	14.6	No heterogeneity dependence
Random Forest regression	0.89	3.8	Strong retention efficiency prediction

The Random Forest model significantly outperforms a baseline, showing that reservoir heterogeneity indicators can successfully predict long-term CO₂ retention performance. The finding from **Table 3** confirms that machine learning model successfully captures the dominant physical controls on storage performance and can reliably predict CO₂ retention in heterogeneous reservoirs.

3.5. Influence of Geochemical Properties on CO₂ Sequestration

Geochemical analysis revealed that basalt, peridotite, and dolerite are the most effective rock types for CO₂ sequestration, with reaction rates of 8.5 - 9.0 kg

CO₂/m³/year and sequestration efficiencies exceeding 85% (Figure 17).

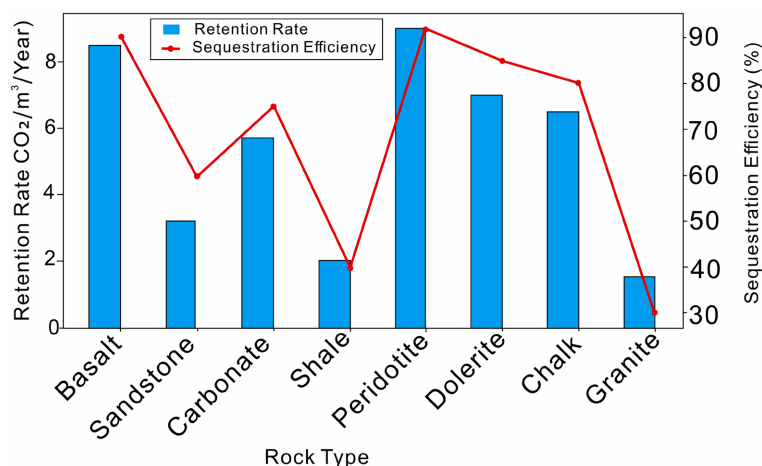


Figure 17. Geochemical sequestration rates and efficiency for different rock types.

Shale and granite, with efficiencies below 50%, were less effective due to lower reactivity and limited porosity.

These results validate earlier studies by [14] [25], and [1], which emphasized the role of mineral composition and geochemical reactivity in long-term CO₂ storage. Studies by [5] and [26] [62] further recommend using geostatistical models to optimize site-specific sequestration. Findings by [3] suggest leveraging advanced monitoring to quantify geochemical reactions in real-time, enhancing predictive modeling accuracy.

Further support comes from studies by [63] and [64], which highlight the interplay between mineral reactivity, pore structure, and fluid dynamics in influencing sequestration outcomes. These insights reinforce the need for integrated approaches to optimize CO₂ trapping while addressing site-specific challenges [65] [66].

The potential for improving geochemical interactions using engineered nanoparticles has been explored in recent studies by [24] [28] and [67]. Nanoparticles, such as functionalized silica, have shown promise in enhancing fluid-rock interactions, thus accelerating mineralization rates and improving trapping efficiency.

3.6. Dynamics of CO₂ Solubility in High- and Low-Permeability Zones

CO₂ solubility dynamics were assessed in high- and low-permeability zones (Figure 18).

High-permeability zones exhibited rapid solubility decline within the first decade, while low-permeability zones maintained higher solubility over time (Figure 18). This behavior highlights the suitability of low-permeability zones for stable, long-term CO₂ storage, as supported by [68].

The study corroborates findings by [13] [69], who noted that restricted CO₂ movement in low-permeability zones enhances dissolution and reduces leakage risks. Studies by [48] [55] and [70] further validate our findings, emphasizing the role of advanced injection strategies in improving solubility retention.

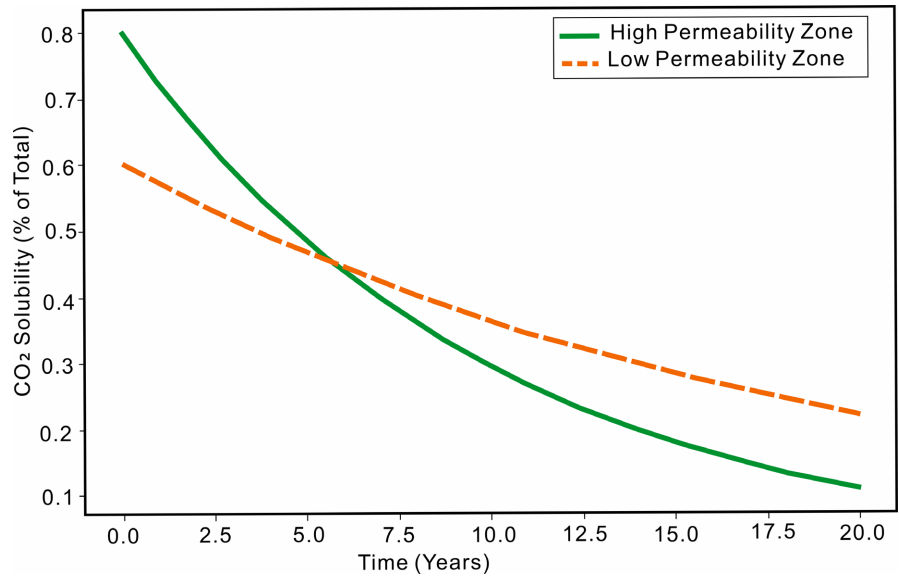


Figure 18. CO₂ solubility dynamics in high- and low-permeability.

3.7. Role of Caprock Integrity and Fault Density in Leakage Risk Assessment

From the risk analysis (Figure 19), several key findings emerged:

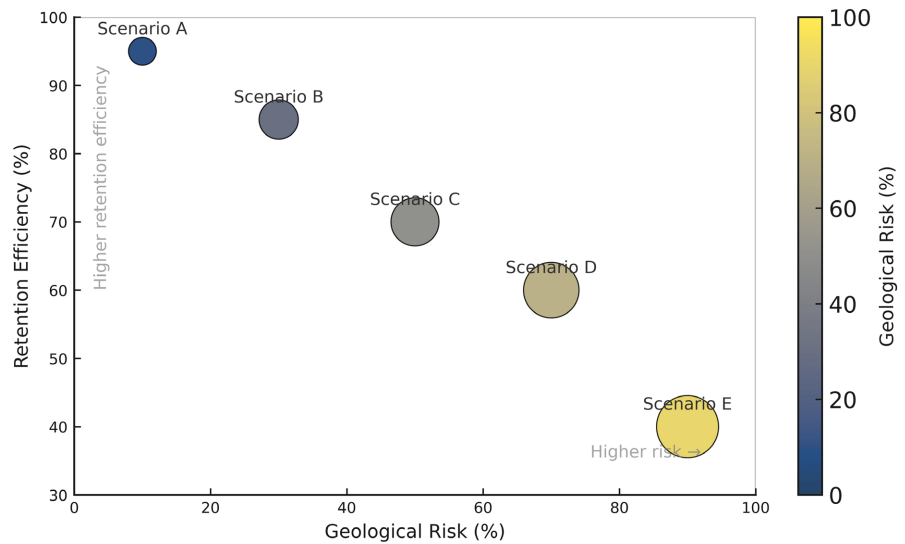


Figure 19. Risk assessment matrix for CCS scenarios.

In this study, five scenarios were analyzed to evaluate the balance between geological risk, retention efficiency, and cost. Scenario A, which represents low geological risk (10%) and high retention efficiency (95%), offers the optimal balance with the lowest cost (1), making it the most favorable option (Figure 19). Scenario B, with a moderate geological risk of 30% and high retention efficiency (85%), has a higher cost (2), reflecting increased complexity or less favorable geological conditions but still provides a viable option (Figure 19). Scenario C, with 50% geo-

logical risk and 70% retention efficiency, has a cost of 3, making it less attractive due to the lower efficiency and higher cost (Figure 19). Scenario D, characterized by a high geological risk of 70% and lower retention efficiency (60%), comes with a cost of 4, marking it as a less desirable option (Figure 19). Finally, Scenario E, with 90% geological risk and very low retention efficiency (40%), is the least favorable due to both its high cost (5) and poor performance, making it the least viable for long-term CCS projects (Figure 19).

These findings align with recent studies emphasizing the trade-off between geological risk, efficiency, and cost in CCS projects [71]-[74], which highlighted the importance of balancing geological risk with retention efficiency for cost-effective CCS, noting that high-risk scenarios incur higher costs, a pattern observed in our study where higher geological risk corresponds to both higher costs and lower retention efficiency. [75] also emphasized this trade-off, pointing out that as geological risks increase, the cost-efficiency curve steepens, a trend seen in our study where higher-risk scenarios are associated with increased costs and reduced retention efficiencies. Our findings suggest that improving the feasibility and sustainability of CCS projects requires efforts to minimize geological risk and maximize retention efficiency [74]. Leakage risk was also modeled as a function of caprock integrity and fault density (Figure 20).

High-risk zones with low caprock integrity ($\leq 30\%$) and high fault density (≥ 8 faults/km²) exhibited leakage probabilities exceeding 80% (Figure 20). In contrast, reservoirs with intact caprocks ($\geq 90\%$) and minimal faulting showed negligible risk (Figure 20).

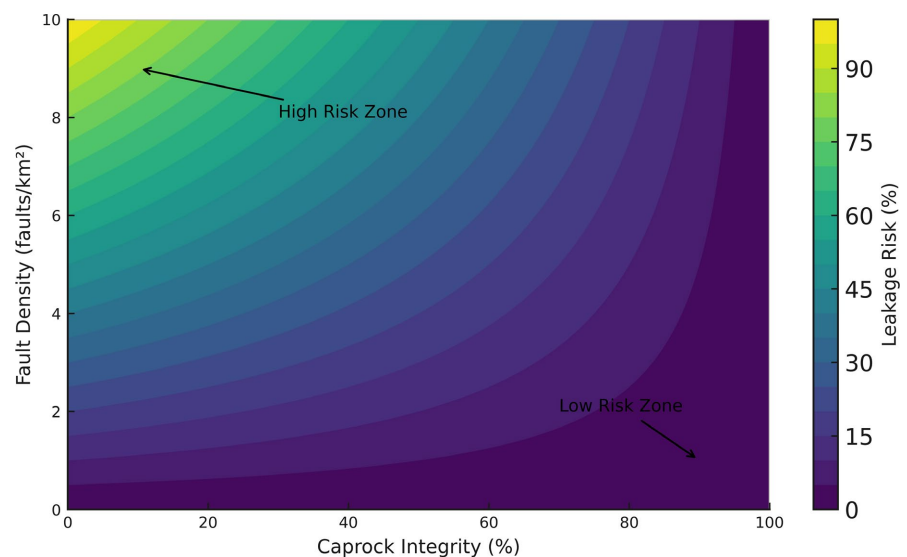


Figure 20. Leakage risk assessment.

These findings align with [35] and [66], emphasizing the importance of robust caprock integrity in preventing CO₂ migration. Advanced sealing techniques and fault management are critical for high-risk scenarios [20]. The economic implications are strongly linked to heterogeneity effects. High-permeability contrast sys-

tems require increased monitoring and pressure management, elevating operational costs. Conversely, basalt formations benefit from rapid mineralization, reducing long-term leakage and surveillance expenditures. These relationships emphasize that geological heterogeneity must be incorporated into early planning for realistic cost-benefit outcomes.

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3.8. Temporal Variability in Residual CO₂ Saturation

Residual CO₂ saturation was compared across reservoirs with varying heterogeneity levels (Figure 21). Highly heterogeneous reservoirs demonstrated slower saturation decay and higher variability, consistent with enhanced capillary trapping. Homogeneous reservoirs exhibited rapid saturation decline, reflecting limited resistance to CO₂ migration (Figure 21). These trends are supported by [76] [77], and [78], who highlighted the influence of geological variability on CO₂ retention.

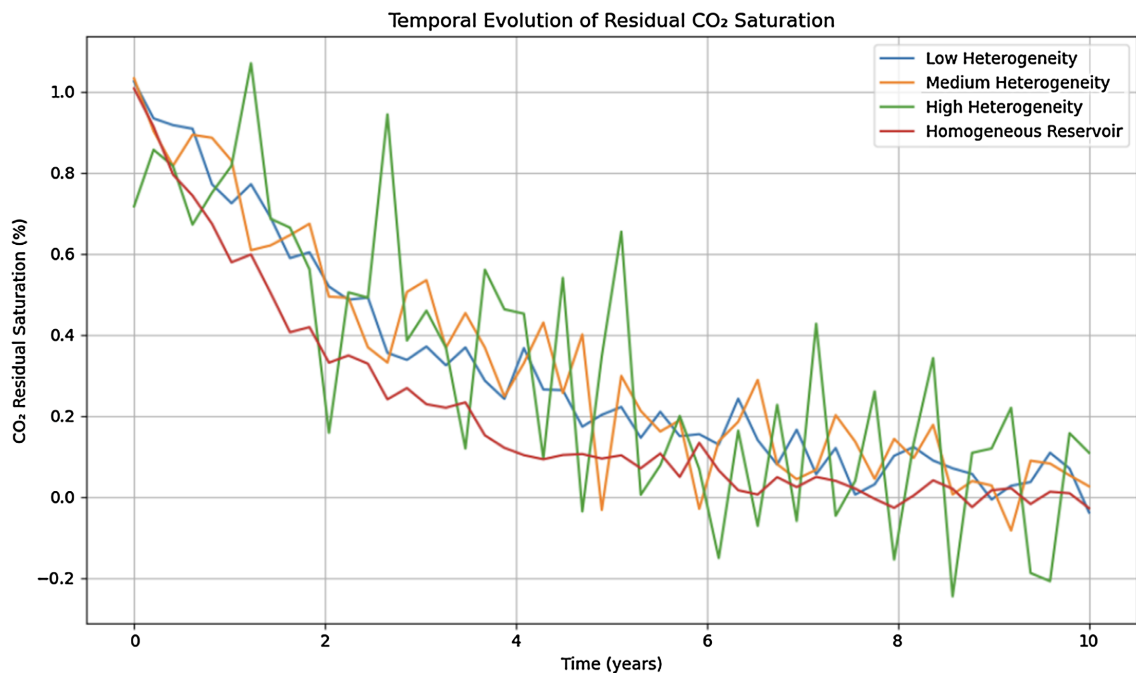


Figure 21. Temporal evolution of residual CO₂ saturation in different reservoir scenarios.

4. Conclusions

This study emphasizes the critical role of reservoir heterogeneity in determining the feasibility and efficiency of carbon capture and storage (CCS) as a climate

mitigation strategy. By analyzing the interactions between geological variability, CO₂ trapping mechanisms, and engineering innovations, it establishes an integrated framework for optimizing CCS performance across diverse geological settings.

The results of this study show that reservoir heterogeneity exerts a dual influence—enhancing residual trapping through capillary barriers while increasing plume migration complexity and potential leakage risks. Basalt formations, with reactive mineralogy and moderate heterogeneity, exhibited the highest mineral carbonation efficiency (92%) and long-term stability, whereas sandstone and carbonate reservoirs showed lower efficiencies, requiring tailored injection and monitoring strategies.

Adaptive injection methods, notably high-pressure pulse and water-alternating-gas (WAG) techniques, improved CO₂ retention and demonstrated the importance of dynamic, site-specific protocols. Caprock integrity and fault stability remained key to storage security, supported by geomechanical modeling and real-time monitoring tools such as distributed acoustic sensing (DAS) and time-lapse seismic imaging.

The integration of machine learning with monitoring systems enabled predictive control of injection parameters, enhancing storage efficiency while reducing leakage risks. Economic analyses identified basalt formations as the most cost-effective option, particularly when coupled with geothermal energy recovery. The integration of machine learning demonstrated that rapid prediction of CO₂ retention performance is achievable using a limited set of heterogeneity descriptors and operational inputs. By quantifying the dominant influence of permeability contrast, the model provides a scalable decision-support tool that can guide injection strategy selection prior to field deployment, reducing both uncertainty and monitoring costs.

Overall, this study provides a comprehensive framework linking geochemical, geomechanical, and data-driven approaches to achieve secure and efficient CO₂ storage. It highlights basalt formations as prime CCS candidates and calls for further exploration of nanotechnology and AI-assisted modeling to advance large-scale, low-risk carbon sequestration.

From a practical standpoint, the results support a decision-making workflow in CCS site development that involves quantifying reservoir heterogeneity through geostatistical modeling, classifying formation type and mineral reactivity, screening compatible injection strategies such as pulse injection in basalt or WAG in sandstone, and defining monitoring intensity based on predicted retention stability. This integrated framework enables CCS operators to align project design with reservoir-specific heterogeneity conditions, thereby improving performance while reducing cost and risk.

Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

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