

Physics-Guided Machine Learning Using Dimensionless Groups to Predict CO₂ Trapping Indices in Deep Saline Aquifers

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ORIGINALITY STATEMENT

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ABSTRACT

Estimating the amount of CO₂ trapped is essential for evaluating the long-term feasibility and security of geological carbon storage (GCS). This study presents a physics-guided machine-learning framework that uses dimensionless groups derived from reservoir and operational parameters to predict the temporal evolution of CO₂ trapping mechanisms in heterogeneous saline aquifers. A conventional reservoir simulator was used to generate 200-year GCS simulation data, and these outputs were transformed into physically meaningful dimensionless inputs to improve model transferability and interpretability. Several machine-learning and deep-learning models were trained and compared for predicting supercritical, dissolved, residually trapped, and mineralized CO₂ fractions. Among the evaluated models, TabM showed the best overall performance, achieving test-set R^2 values of 0.957, 0.964, 0.942, and 0.930 for supercritical, dissolved, residually trapped, and mineralized CO₂, respectively, with similarly strong 5-fold cross-validation R^2 values of 0.943, 0.942, 0.933, and 0.938. Symbolic regression was further used to derive explicit closed-form equations for the trapping indices, which provides interpretable predictive equation. Shapley Additive Explanations (SHAP) were applied to quantify feature importance and identify the dominant controls for each trapping mechanism. Dissolved CO₂ was governed mainly by brine salinity and injected pore volume, residual trapping was controlled primarily by residual gas saturation and storage time, and mineral trapping was influenced most strongly by storage duration and temperature. For supercritical CO₂, injection period and brine salinity were found to be the main controls, while buoyancy-related effects were a secondary role. Beyond prediction, the TabM model was applied to Monte Carlo analysis, sensitivity analysis, and inverse-design optimization. High-performing cases were associated with intermediate-to-high PV injected, moderate dimensionless drawdown, moderate heterogeneity, limited residual gas immobilization, and relatively high gravity number, temperature, and salinity. These trends indicate that optimal mineral trapping is controlled by a balanced combination of flow, storage, and reservoir-condition parameters. Overall, the proposed framework provides a computationally efficient alternative to repeated full-physics simulations and offers a practical basis for rapid screening, sensitivity assessment, and recommended operating ranges for CO₂ storage in heterogeneous saline aquifers.

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1. INTRODUCTION

1.1 Background

Since the Industrial Revolution, heavy dependence on fossil fuels has significantly increased atmospheric greenhouse gas concentrations. This rise has been linked to major environmental impacts, including global warming, climate change, and ocean acidification. Among the main greenhouse gases, CO₂ is considered the most important due to its high atmospheric concentration and strong contribution to radiative forcing. Recent data show that the mean atmospheric CO₂ concentration increased from 399.65 ppm in 2015 to 427.35 ppm in December 2025, indicating the continuing growth of global emissions and their increasing effect on the Earth's climate system (**Figure 1**)¹. To address this challenge, international efforts have focused on limiting temperature rise and reducing greenhouse gas emissions. A key milestone was the Paris Climate Agreement, which set the goal of restricting global mean temperature increase to 1.5 °C above pre-industrial levels². However, global demand for fossil fuels remains high, which limits the transition to low-emission technologies^{3,4}. Therefore, additional mitigation strategies are needed, and carbon capture and storage (CCS) has become an important option for supporting global decarbonization efforts^{5,6}.

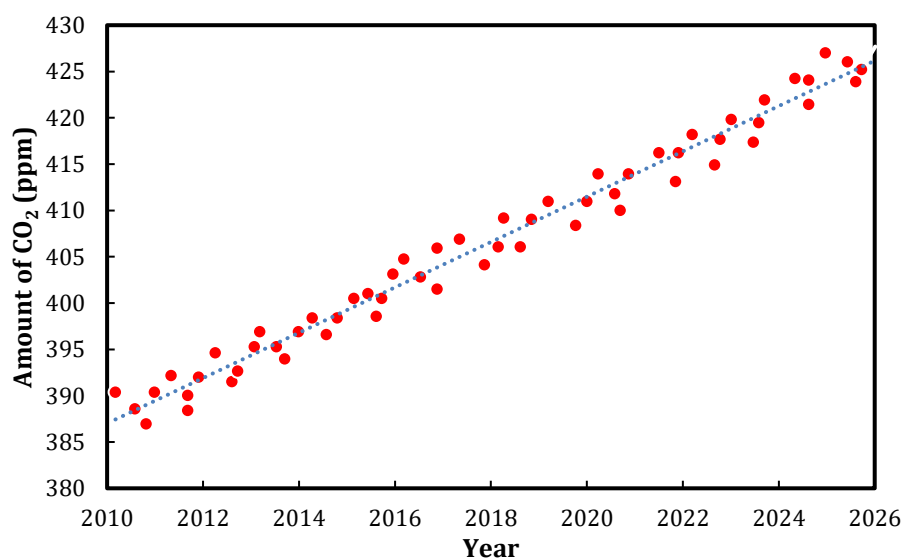


Figure 1. Mean amount of CO₂ in atmosphere. Data from¹.

Geological carbon storage (GCS) is a key part of CCS because it enables long-term isolation of captured CO₂ in deep subsurface formations instead of releasing it to the

atmosphere⁷. Proposed storage options include deep saline aquifers^{8–11}, depleted and existing oil and gas reservoirs^{12–16}, unmineable coal seams^{17–20}, basalt formations²¹, organic-rich shales^{22–26}, and CO₂ hydrate storage systems^{27–29}. Deep saline aquifers are generally considered the most practical because of their wide distribution and high storage^{13,30}. In most cases, storage takes place in porous sandstone or carbonate formations sealed by low permeability caprock that helps prevent upward CO₂ migration^{31–33}.

After injection, CO₂ storage security depends on the trapping mechanisms that prevent leakage. In deep saline aquifers, the main trapping mechanisms are structural, dissolution trapping, capillary or residual trapping, and mineral trapping¹³. Structural and residual trapping are mainly considered the most influential mechanisms during the early period of a storage project. Dissolution and mineral trapping become more important over longer time scales^{13,34}. Because buoyant CO₂ can migrate through faults, fractures, or artificial pathways such as wells, a thorough assessment of trapping behavior is essential for storage-site selection^{35,36}.

To evaluate these coupled processes, numerical simulation has become one of the main tools in geological CO₂ storage research and design. Such modeling typically requires extensive geological and petrophysical input data, including reservoir framework, rock properties, and formation characterization³⁷. In saline aquifers, simulation is particularly important because storage performance depends not only on reservoir capacity but also on the behavior of the major trapping mechanisms, especially structural, residual, solubility, and mineral trapping^{13,38,39}. For this reason, field-scale compositional reservoir simulations have been widely applied to estimate CO₂ trapping efficiency in deep saline aquifers^{40–44}.

Although simulation-based approaches are essential for evaluating CO₂ storage performance, they are computationally demanding and require large amounts of subsurface data, which is usually expensive and difficult to obtain^{45,46}. These limitations become more significant when long-term prediction, reservoir heterogeneity, and uncertainty analysis are involved, making rapid screening difficult with conventional high-resolution models. For this reason, several studies have explored machine learning as an alternative or complementary approach for predicting CO₂ trapping behavior^{45–47}. Nevertheless, most existing ML models are based on dimensional input variables, and only limited models can simultaneously predict multiple trapping mechanisms. Given its speed and predictive capability, ML offers strong potential for efficient storage assessment.

1.1 Objectives of the Thesis

1.1.1 Main Objectives

The main objective of this thesis is to develop a physics-guided machine learning framework to predict the temporal evolution of CO₂ trapping mechanisms in heterogeneous deep saline aquifers with dimensionless numbers derived from reservoir and operational parameters. The study aims to provide a computationally efficient and physically interpretable model rapid screening, sensitivity analysis, and assessment of geological CO₂ storage performance.

1.1.2 Specific Objectives

The specific objectives of this thesis are as follows:

1. To construct a numerical simulation dataset for deep saline aquifer CO₂ storage in the CMG-GEM simulator combined with CMOST under a wide range of reservoir, operational, and heterogeneity conditions.
2. To quantify the main CO₂ trapping mechanisms, such as supercritical, solubility, residual, and mineral trapping, over a long-term simulation period.
3. To transform the original input variables into physically meaningful dimensionless groups that capture the dominant controls on CO₂ migration and trapping.
4. To develop and compare different machine-learning models for predicting CO₂ trapping indices based on the engineered dimensionless features.
5. To identify the best-performing predictive model and evaluate its performance using appropriate statistical metrics.
6. To derive explicit predictive equations through symbolic regression to improve model interpretability and practical applicability.
7. To analyze the relative importance of the input features governing each trapping mechanism using explainable artificial intelligence methods.

1.2 Scope of Work

This thesis focuses on the prediction of CO₂ trapping indices in deep saline aquifers through the integration of numerical reservoir simulation and machine learning. A three-dimensional radial aquifer model was developed in CMG-GEM to simulate multiphase flow and reactive transport during CO₂ injection and post-injection periods. The analysis considered variations in key reservoir and operational parameters, including pressure, temperature, salinity, reservoir thickness, injection rate, residual gas saturation, permeability, porosity, and heterogeneity represented by the Dykstra–Parsons coefficient. Based on the simulation outputs, a dataset was generated and used to construct dimensionless input features such as gravity number, injected pore volume, and pressure drawdown. These features were then applied to train and evaluate several machine-learning models for predicting supercritical, dissolved, residual, and mineralized CO₂ fractions. The scope of this work also includes symbolic regression for obtaining closed-form predictive equations and SHAP-based interpretation of feature importance. However, the study is limited to the geological, physical, and geochemical conditions represented in the simulation dataset and does not explicitly include complex structural features such as faults and fractures or validation against field-scale operational data.

2. LITERATURE REVIEW

This chapter presents a critical review of the literature on geological CO₂ storage in deep saline aquifers. Deep saline aquifers have attracted significant attention as secure long-term storage formations due to their high storage potential and widespread occurrence. The chapter begins with a description of the fundamentals of carbon capture and storage and the importance of geological sequestration. It then reviews the main geological storage options and explains why saline aquifers are considered a particularly suitable target for large-scale storage.

The four principal trapping mechanisms are then examined, along with the geological and operational factors that control their efficiency. In addition, the chapter summarizes current numerical and machine learning approaches that are used for assessing storage performance and highlights the limitations of current studies.

2.1 Physicochemical properties of CO₂

Carbon dioxide is a simple molecular compound composed of one carbon atom and two oxygen atoms connected by double covalent bonds ⁴⁸. Under ambient surface conditions, it exists mainly in the gaseous state, but its phase varies with pressure and temperature, as shown in **Figure 2** ⁴⁹. Critical point is located at 304.2 K and 73.9 bar; beyond this point, CO₂ enters the supercritical region ⁵⁰. In the supercritical state, CO₂ combines relatively high density with favorable flow characteristics ^{51,52}. Because both pressure and temperature increase with burial depth, injected CO₂ commonly transitions into this state in deep geological formations, mainly at depths greater than about 800 m ^{53,54}.

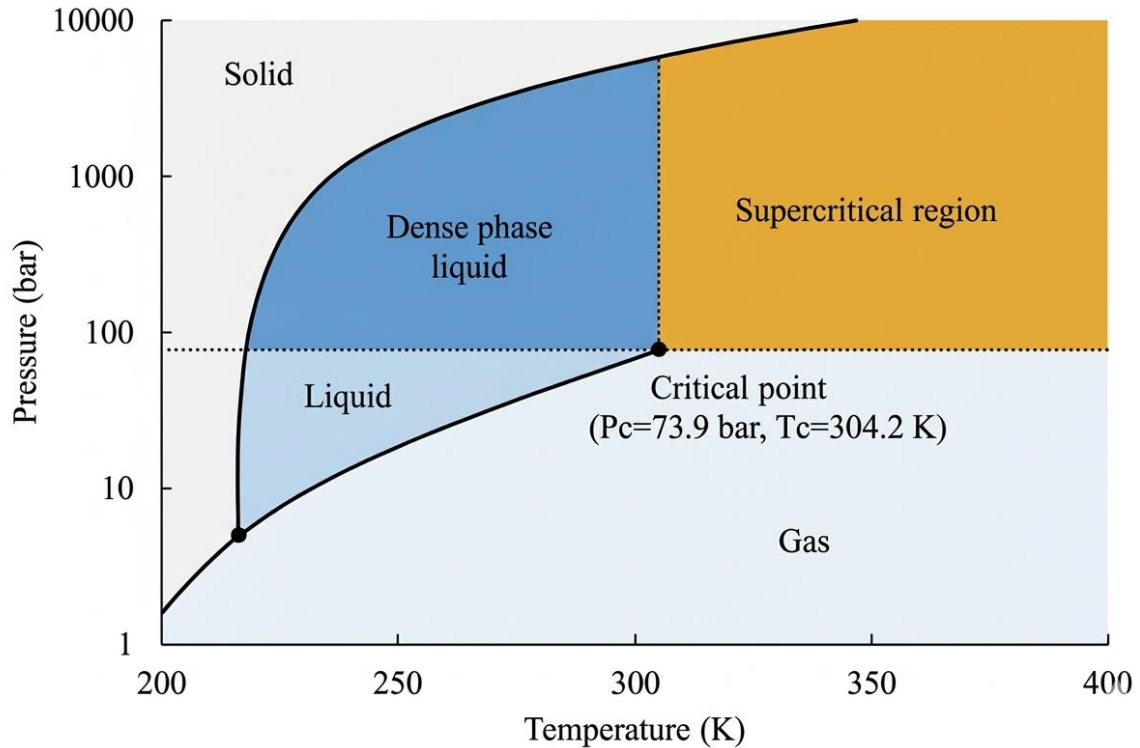


Figure 2. Pressure-temperature phase diagram of CO₂. It shows its major phase regions, such as the supercritical region above the critical point. Adapted from ⁴⁸.

2.2 Carbon Capture and Storage

Carbon capture and storage (CCS) is widely regarded as one of the most important approaches to reduce CO₂ emissions. CCS is based on the principle of capture of greenhouse gases from both stationary sources, such as power plants, and mobile sources, such as automobiles, followed by their storage in geological formations^{55,56}. Emissions from stationary sources are estimated to be about 13 billion tons annually, whereas nonstationary sources contribute approximately 2.5 billion tons per year⁵⁷.

The CCS process is commonly divided into four main stages: capture, compression, transport, and injection⁵⁸. In this process, CO₂ is separated from major emission sources such as power plants, coal-fired facilities, or industrial plants. It is then compressed to reduce its volume and prepare it for transportation.⁵⁹ The compressed CO₂ is subsequently injected into carefully selected geological formations under controlled conditions. In addition, CCS requires careful measurement and monitoring to ensure that the injected CO₂ remains securely stored for long periods without leaking back to the surface⁶⁰. Therefore, these site-specific factors are

usually evaluated through screening studies, pilot tests, and numerical assessment before field deployment^{61,62}. **Table 1** presents representative geological CO₂ storage projects and their main storage characteristics.

Table 1. Summary of different geological CO₂ storage projects, their storage capacities, geological settings, reservoir formations or caprocks, and references.

Project and location	Reported storage estimate	Storage setting	Reservoir formation	References
Sleipner, Norway	25 million tonnes (Mt)		Sandstone	63,64
Rangely, USA	25 Mt		Sandstone	65
Gorgon Field, Australia	129 Mt		Sandstone, siltstones	66
Nagaoka Field, Japan	128 Mt	Deep saline aquifer	Sandstone	67
Ketzin, Germany	67,271 t of CO ₂		Sandstone	68
Ordos, China	~0.15 Mt in 2014		Sandstone	63
In Salah, Algeria	~ 17 Mt of CO ₂ between 2004 and 2011		Sandstone	63,69
Carbfix, Iceland	Expected injection of 2.2 Mt		Basalt	70
Wallula Basalt Project, Columbia	10–50 Gt CO ₂	Basalt	Basalt	71
Cranfield, USA	5 Mt		Sandstone	63
SACROC Field, USA	255 Mt injected and 100 Mt stored	Depleted hydrocarbon reservoir	Limestone carbonate	66
Weyburn, Canada	Approximately 20 Mt of CO ₂ by 2030		Carbonate	72

2.3 Geological Carbon Storage options

Among the available CCS pathways, geological carbon storage (GCS) has emerged as a major option for storage of large quantities of captured CO₂ due to its very large theoretical

capacity and strong potential for long-term subsurface containment. CO₂ sequestration projects are already in operation in regions such as the United States and northern Europe, and similar initiatives have recently expanded across countries including China, South Korea, Japan, New Zealand, and Australia ^{73–75}. Geological assessments suggest that the global storage capacity for CO₂ may lie in the range of 8,000 to 55,000 Gt, which indicates that subsurface sequestration could play a substantial role in long-term carbon management strategies ⁷⁶. The feasibility of this approach is supported by the natural ability of subsurface formations to confine fluids such as hydrocarbons and water over millions of years. This long-term containment is primarily controlled by impermeable caprock layers, which serve as hydromechanical barriers against upward CO₂ migration ^{38,77}. Moreover, capillary and viscous resistance at the reservoir–caprock boundary can further limit leakage, even under injection-related pressure buildup ⁷⁸.

GCS can be implemented in several types of subsurface formations, each characterized by distinct storage mechanisms, advantages, and technical constraints. The suitability of a given storage option depends on properties such as porosity, permeability, sealing capacity, depth, geochemical reactivity, and structural integrity. Among the most widely studied options are saline aquifers, depleted oil and gas reservoirs, unmineable coal seams, basalt formations, and CO₂ hydrate-based storage systems. Although all of these formations offer potential for long-term CO₂ sequestration, they differ in terms of storage behavior, maturity of development, economic feasibility, and containment mechanisms. **Figure 3** compares the estimated storage-capacity ranges of major geological CO₂ sequestration options. Deep saline formations show the largest overall storage potential, which makes them the most promising option for large-scale CO₂ storage. Depleted oil and gas reservoirs also provide substantial capacity, whereas coal seams, CO₂-EOR, and organic-rich shales generally show lower or more limited potential. However, despite their high capacity, saline formations remain difficult to characterize, while coal seams are particularly challenging for CO₂ injection because of their very low permeability.

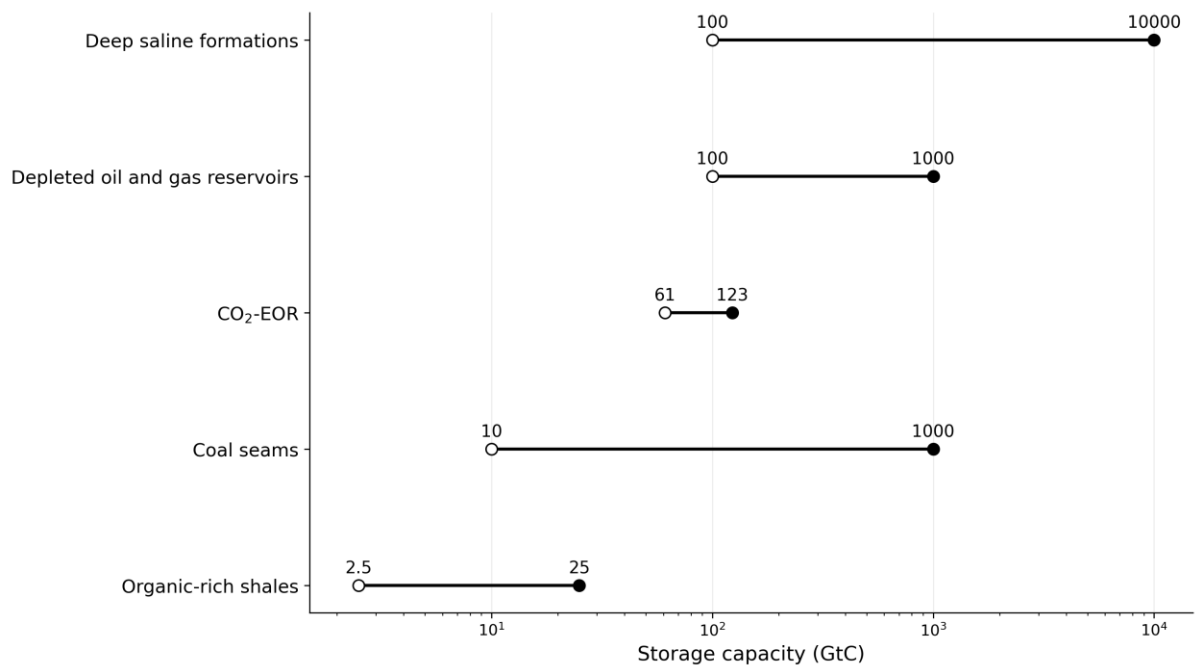


Figure 3. Estimated storage-capacity ranges of major CO₂ sequestration options shown on a logarithmic scale. Open circles represent the minimum estimated storage capacity, while filled circles indicate the maximum estimated storage capacity ⁷⁹.

2.2.1 Deep saline aquifers

Deep saline aquifers are among the most extensively investigated and widely available options for geological CO₂ storage. These formations consist of porous and permeable reservoir rocks whose pore spaces are saturated with saline water, typically at depths below potable groundwater systems ⁸. Their broad geographic occurrence, favorable geological characteristics, and large theoretical storage capacity make them one of the most attractive candidates for long-term CO₂ sequestration ^{9–11}. Suitable saline aquifers are commonly located at depths of about 800 to 3000 m, where the pressure–temperature conditions allow injected CO₂ to remain in a dense supercritical state ^{10,80}. Historically, one of the earliest and most well-known saline aquifer storage projects was conducted at Sleipner in the North Sea, where CO₂ was injected into the Utsira Sandstone Formation ⁸¹.

From a geological standpoint, saline aquifers are often composed of porous sedimentary rocks, particularly sandstone and carbonate formations, which improves both CO₂ injection and migration within interconnected pore networks ^{80,82–84}. Their storage potential can be very large; for example, long-term storage capacity values of approximately 30 kg/m³ have been reported for some saline aquifer systems, while global estimates suggest that these formations

may store up to 10,000 Gt of CO₂ ^{85,86}. An additional advantage of saline aquifers is that, after injection, dissolved CO₂ may react with formation water and minerals to generate more stable mineral phases ¹². Moreover, overburden impermeable caprock acts as a barrier that prevents upward migration of CO₂ ⁸⁷. Due to this combination of storage volume, broad occurrence, and multiple trapping mechanisms, saline aquifers are often considered as the most preferred option for large-scale CO₂ storage.

2.2.2 Depleted oil and gas reservoirs

Depleted hydrocarbon reservoirs are other potential candidates for geological CO₂ storage. These formations are generally well characterized, because they have been extensively studied in the production stage¹². Available geological information is a major advantage, because it reduces uncertainty about storage performance. Depleted oil and gas reservoirs are considered particularly attractive because they have naturally accumulated hydrocarbons over geological timescales, which demonstrates that they have the most important structural and sealing conditions necessary for fluid trapping ¹⁶.

Nevertheless, despite these benefits, depleted hydrocarbon reservoirs are not without risk. Their long production history may have altered reservoir pressure, mechanical condition, and fault stability, and legacy wells may create potential leakage pathways if not properly assessed and addressed. Even so, because of their known geology, demonstrated containment capability, and infrastructure advantage, depleted oil and gas reservoirs remain one of the practical and technically mature GCS options.

2.2.3 Unmineable coal seams

Deep coal seams that are not economically or technically suitable for mining have also been proposed as storage formations for CO₂ sequestration ¹⁷. Unlike saline aquifers or depleted hydrocarbon reservoirs, CO₂ storage in coal seams is governed primarily by adsorption rather than by simple pore-space occupation ²⁰. When injected into a coal seam, CO₂ molecules preferentially adsorb onto the internal coal surface, which leads to the formation of an adsorbed phase rather than free fluid in interconnected pores. This distinction makes coal seams a unique storage medium within the broader range of GCS options. Reported storage estimates illustrate their potential significance; for example, deep coalbeds in Alberta, Canada,

have been estimated to hold approximately 20 Gt of CO₂, while Dutch coal seams have been projected to store around 8 Gt ^{88,89}.

2.2.4 Basalt formations

Basalt formations recently have attracted more attention as a geological storage option because of their strong potential for mineral trapping. Basalt is an igneous rock formed by the solidification of molten lava, and its minerals make it highly reactive with CO₂-bearing fluids ²¹. In basalt storage systems, the dominant storage mechanism is mineral carbonation. Once CO₂ is injected into the formation, it can react with divalent cations such as calcium, magnesium, and iron to produce stable carbonate minerals, such as calcite, magnesite, and siderite ⁹¹. Because of this strong mineralization potential, basalt formations have become a major focus of research in recent years ^{92–96}. An important advantage of basalt storage is that the precipitated carbonate minerals are environmentally stable and can remain securely stored over extremely long periods.

2.2.5 Hydrate-based CO₂ storage

Another geological storage concept includes the formation of CO₂ hydrates under specific pressure and temperature conditions. In this approach, CO₂ interacts with water to form a crystalline hydrate structure in which CO₂ molecules are physically trapped within cage-like water frameworks ²⁸. Unlike mineral trapping, the CO₂ in hydrates is not chemically bonded but is instead held within a stable solid structure maintained by surrounding water molecules ^{99,100}. This storage mechanism is particularly relevant in deep marine sediments and permafrost regions, where the pressure–temperature environment is favorable for hydrate stability. Because CO₂ hydrate is dense, the amount of CO₂ that can be stored within a given hydrate-bearing volume may exceed that achievable under gaseous or even supercritical storage conditions ^{101,102}.

Hydrate-based sequestration is primarily viewed as a long-term storage option, provided that the environmental conditions required for hydrate stability remain undisturbed ¹⁰². In addition, this concept has attracted interest in enhanced gas recovery applications, where CO₂ may replace methane in naturally occurring gas hydrates, allowing methane to be produced while CO₂ remains trapped in hydrate form ²⁹.

Despite these benefits, hydrate storage remains more condition-sensitive than conventional storage in saline aquifers or depleted reservoirs. Its success depends strongly on local subsurface thermodynamic conditions. Therefore, although it offers high-density storage and interesting recovery synergies, hydrate-based sequestration is still less mature than other major GCS options. **Figure 4** illustrates the principal geological carbon storage options.

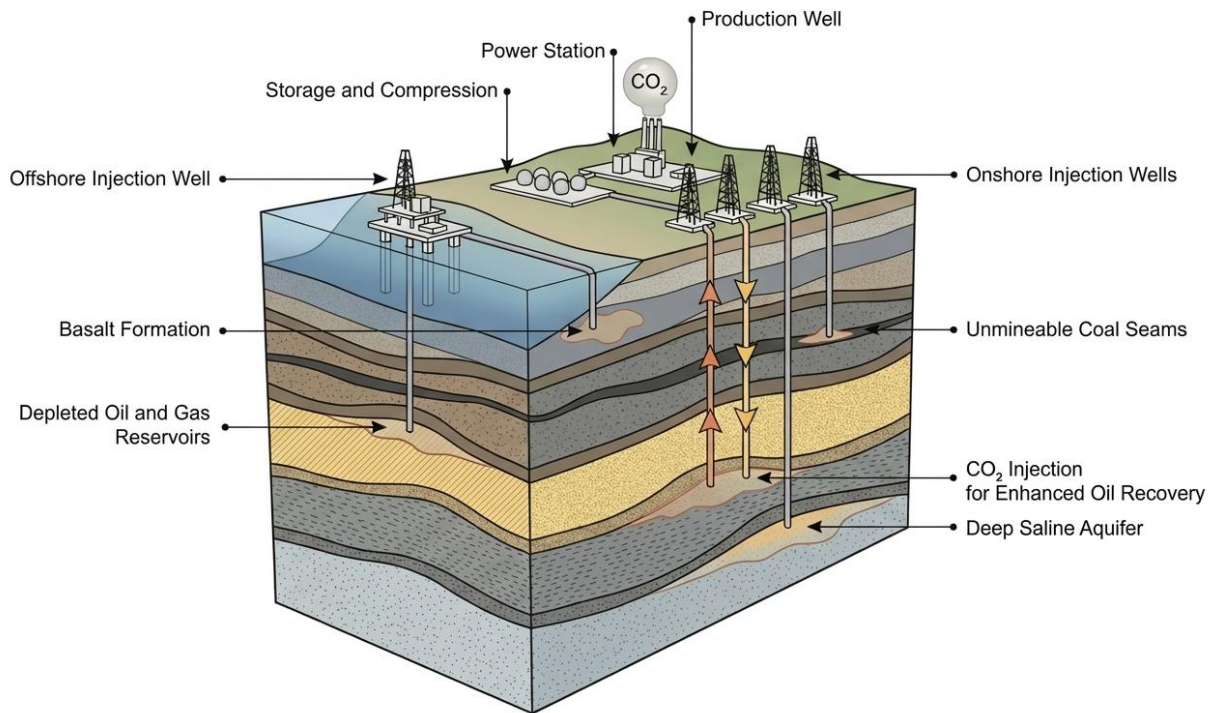


Figure 4. Schematic illustration of major geological carbon storage options. Modified from ³⁸.

Despite the choice of storage reservoir, effective GCS requires several common formation characteristics. Appropriate storage formation should have enough pore space to store a feasible amount of CO₂, and it should also have sufficiently high permeability to allow for injection and CO₂ plume migration within the reservoir ^{103,104}. Sedimentary basins, such as sandstones and carbonates, often possess such characteristics. For this reason, such formations have become primary targets for CO₂ storage. Another important factor is the presence of an impermeable caprock, which serves as a barrier that prevents upward CO₂ migration and leakage. The caprock must be mechanically and chemically stable, as CO₂ injection additionally increases reservoir pressure, and it should also withstand tectonic stress conditions ¹⁰⁷.

Deep saline formations are widely regarded as one of the most practical options for large-scale CO₂ storage because of their broad distribution and substantial storage potential. In addition, the highly saline nature of the formation water makes these aquifers unsuitable for drinking water, agricultural irrigation, and most industrial uses. A significant share of the projected storage potential is located onshore within depleted fields and deep saline formations, although offshore systems also offer considerable capacity, estimated at 2000 to 13,000 Gt ¹¹⁵.

2.3 Trapping mechanisms in deep saline aquifers

The effectiveness and long-term reliability of geological CO₂ storage depend on the trapping processes that keep injected CO₂ within the subsurface and prevent its upward migration. These retention processes act together to isolate CO₂ from the atmosphere and are therefore fundamental to the viability of CCS as a large-scale emission reduction strategy ⁷⁹. In general, CO₂ trapping mechanisms in geological formations are classified into physical and chemical categories, with the main mechanisms commonly classified as structural or stratigraphic trapping, capillary or residual trapping, solubility trapping, and mineral trapping ¹³.

As illustrated in **Figure 5**, the relative contribution of these mechanisms evolves over time after injection stops: structural and stratigraphic trapping dominates at the early stage, whereas residual, solubility, and mineral trapping become more important over longer time. Additional retention processes, such as adsorption and ionic exchange, may also occur in certain formations, although their contribution is usually more site-specific ¹¹⁷. Since buoyant CO₂ may migrate upward and potentially escape through natural discontinuities such as faults and fractures or through artificial pathways such as wells, a clear assessment of these trapping processes is essential for evaluating storage security ³⁵. Their relative importance depends on formation type, physicochemical conditions, and the time scale of storage, which is why thorough assessment of trapping behavior is central to the selection and safe operation of geological CO₂ storage sites ³⁴.

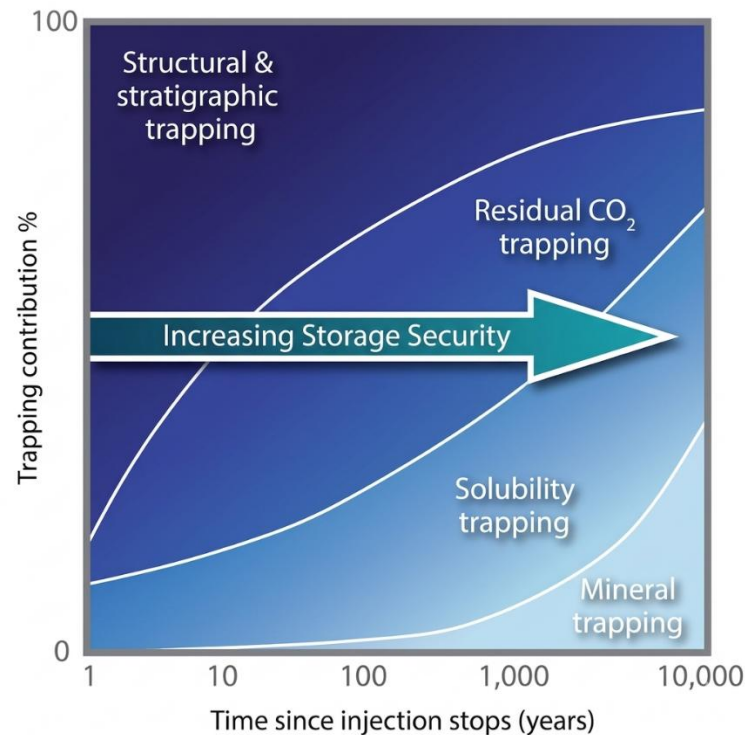


Figure 5. Temporal evolution of the main CO₂ trapping mechanisms in geological storage after injection stops, indicating the growing contribution of residual, solubility, and mineral trapping and the corresponding increase in storage security over time. Redrawn from ¹³

2.4.1 Structural/Stratigraphic trapping

Stratigraphic and structural trapping are the earliest and most immediate forms of CO₂ retention in many geological storage systems, because they restrict the movement of buoyant CO₂ before the contribution of other trapping mechanisms becomes significant. Stratigraphic trapping occurs where depositional architecture, lithological variation, or diagenetic alteration creates laterally or vertically continuous barriers to fluid migration. In such cases, contrasts in permeability and capillary entry pressure between adjacent rock units can restrict CO₂ flow even in the absence of a large four-way structural closure, which leads to plume confinement within specific stratigraphic intervals ¹¹⁸. Structural trapping is associated with geometrical closures produced by deformation, where injected CO₂ rises through the reservoir under buoyancy forces until it is blocked by caprock ^{35,119}.

Different sealing styles have been identified in such settings, including cataclastic fault rocks, juxtaposition seals, cemented fault zones, phyllosilicate-rich fault rocks, and clay smears ⁴⁸. Fold-related trapping is also important, especially in anticlines and dome-shaped structures formed during tectonic deformation, where the geometry naturally promotes fluid

accumulation beneath a fine-grained sealing layer such as shale or mudstone ^{121,122}. As illustrated in **Figure 6**, structural-stratigraphic trapping may therefore occur in both fault-bounded reservoirs and folded anticline closures, where buoyant CO₂ accumulates beneath an impermeable seal.

The performance of structural and stratigraphic trapping is closely tied to caprock quality. During and after injection, CO₂ tends to move upward because it is less dense than the formation fluids. This upward migration can be blocked at the reservoir-caprock boundary if the seal has sufficiently low permeability and a capillary entry pressure greater than the buoyancy pressure exerted by the trapped CO₂ column ^{35,123}. In practical terms, caprock must not only resist fluid flow but also maintain adequate mechanical strength under injection-induced stress changes to preserve long-term storage ^{124–127}. If the buoyancy pressure remains below the capillary threshold, CO₂ can accumulate safely beneath the seal; however, once that threshold is exceeded, CO₂ may be forced through pore throats or discontinuities in the caprock, increasing leakage risk ¹²³.

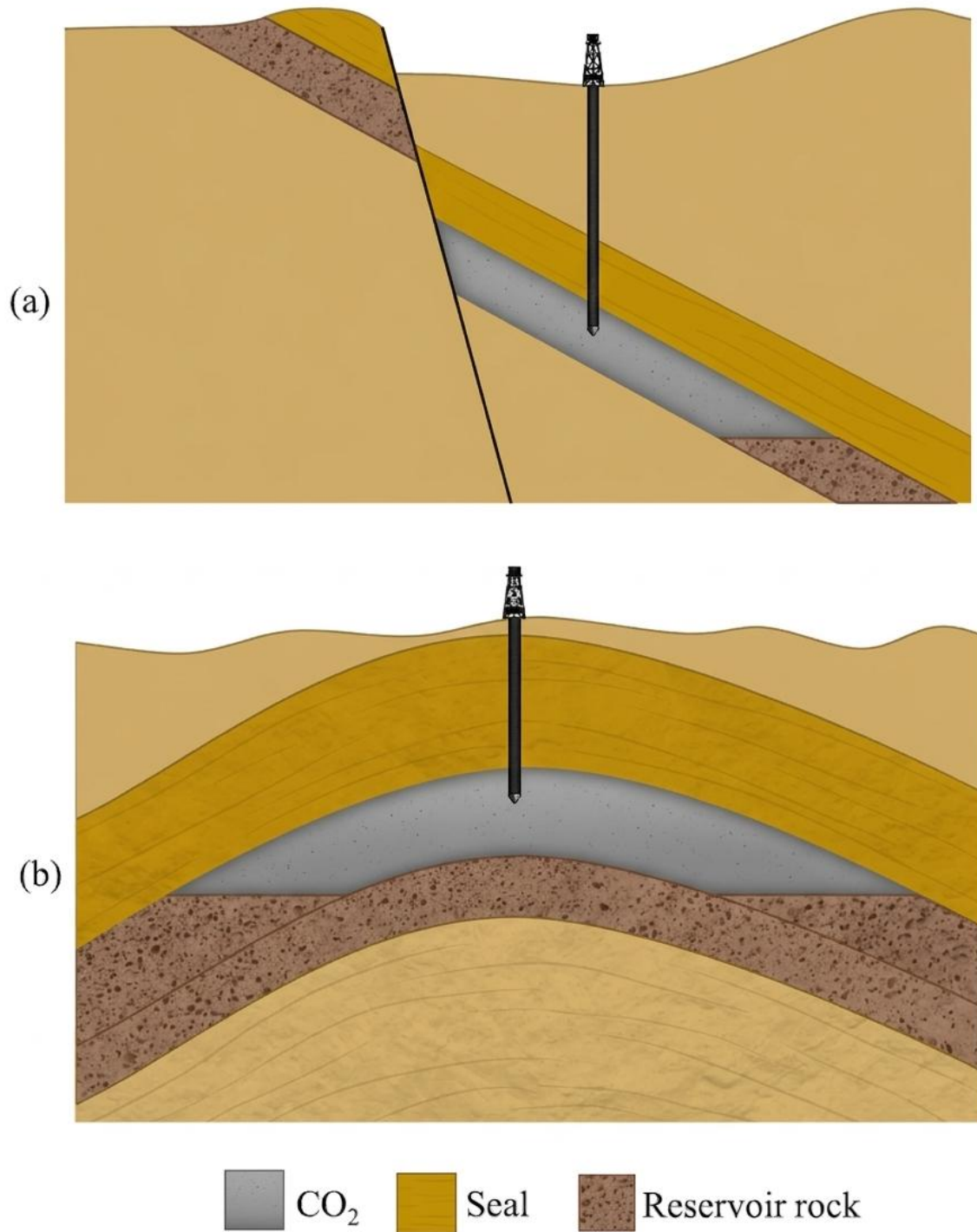


Figure 6. Schematic illustration of structural and stratigraphic CO₂ trapping: (a) trapping in a fault-bounded inclined reservoir beneath an impermeable seal, and (b) trapping in an anticline structure where CO₂ accumulates below the caprock. Redrawn from ⁴⁸

2.4.2 Residual (capillary) trapping

Residual trapping is a major mechanism that immobilizes CO₂ after it is injected into a brine-saturated formation. During drainage, CO₂ behaves as the non-wetting phase and displaces brine from the pore space. When injection declines or ceases, brine re-enters the formation during imbibition and fragments the continuous CO₂ phase into isolated droplets, ganglia, and small clusters that are held in place by capillary forces^{128–130}. This process is illustrated in **Figure 7**. This occurs because buoyancy is insufficient to overcome capillary entry pressure at pore throats, which prevents the disconnected CO₂ from the upward movement. Unlike structural trapping, this mechanism can keep CO₂ below or beyond structural closures without dependence on caprock^{128,131,132}.

The extent of residual trapping is governed by the interaction between drainage and imbibition. CO₂ invasion continues until the rock approaches irreducible water saturation and maximum CO₂ saturation, after which returning brine reduces CO₂ mobility until its relative permeability approaches zero. Irreducible water saturation is especially important because it restricts the pore volume available for CO₂ storage; accordingly, lower irreducible water saturation generally allows more CO₂ to remain trapped. The trapped amount is further controlled by wetting and non-wetting phase behavior, which influences capillary pressure and relative permeability¹³⁶. Residual CO₂ saturation also depends on multiple rock and fluid properties, including lithology, wettability, pore aspect ratio, pore geometry, hysteresis, impurities in the CO₂ stream, CO₂ viscosity, interfacial tension, initial fluid saturation, porosity, pore pressure, flow rate, gravity number, capillary number, and coordination number^{129,137}. In consolidated formations, lower porosity has also been associated with greater residual CO₂ saturation¹³⁸.

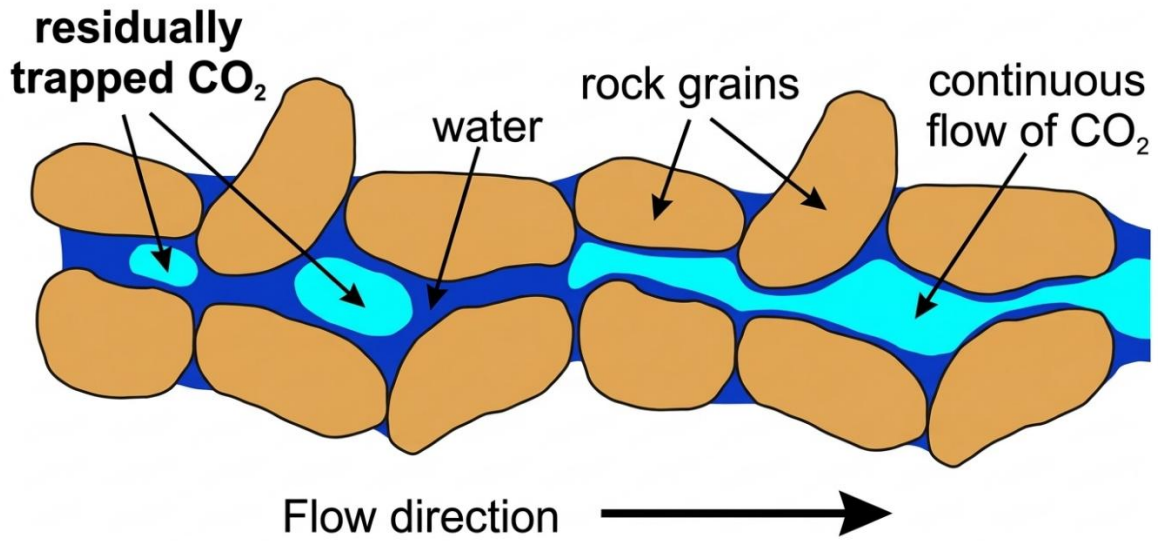
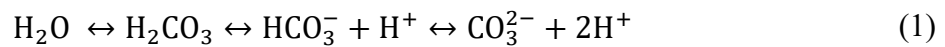


Figure 7. Conceptual illustration of residual trapping at the pore scale, where imbibing water disconnects the non-wetting CO₂ phase into isolated ganglia that remains immobilized between rock grains by capillary forces.

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2.4.3 Solubility trapping

Solubility trapping takes place when injected CO₂ dissolves into reservoir brine and is converted from a separate mobile phase into dissolved aqueous species. This reduces the possibility of leakage as free CO₂ because the dissolved fraction no longer exists as a discrete buoyant phase. In the aqueous system, dissolved CO₂ is present through a series of reactions that generate carbonic acid, bicarbonate, and carbonate species. The overall dissolution represented in **Equation (1)**¹³:

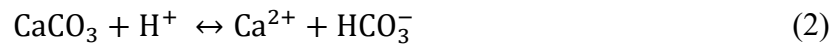


The extent and rate of this process depend on several reservoir and fluid properties, which include permeability, porosity, CO₂ flow rate, and the effective diffusion coefficients¹³⁹. Temperature and brine salinity are also major controls, and CO₂ solubility generally declines as either of these increases. Dissolution is usually fastest when CO₂ first contacts unsaturated brine, but once the brine becomes enriched in dissolved CO₂, the rate slows and is then governed mainly by diffusion¹³. In addition, dissolution slightly increases brine density, so CO₂-rich brine may sink under gravity, which improves convective mixing as shown in **Figure 8**. This behavior helps suppress upward CO₂ migration and can increase the storage capacity of the formation^{7,102,140}

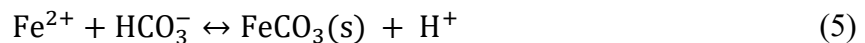
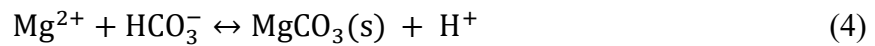
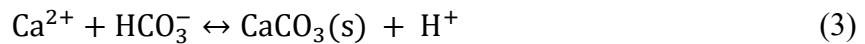
2.4.4 Mineral trapping

Mineral trapping refers to the formation of stable solid minerals from injected CO₂ through long-term geochemical reactions. Among the major trapping mechanisms, it is the slowest and the most permanent form of CO₂ trapping¹⁴¹. The process begins after CO₂ dissolves in brine and forms carbonic acid, which increases fluid acidity of initial brine. This reaction releases cations into the brine and generates bicarbonate species. These species create the chemical conditions required for subsequent mineral precipitation^{142,143}. On geological timescales, this sequence transforms dissolved CO₂ into stable minerals. The geochemical pathway of mineral trapping can be represented through a sequence of dissolution and precipitation reactions.

First, dissolved CO₂ forms carbonic acid and dissociates in the aqueous phase. The acidic fluid then reacts with reservoir minerals and releases dissolved cations. These reactions are shown in **Equations (2)-(5)**:



These cations can later combine with bicarbonate to precipitate carbonate minerals, such as:



Mineral trapping strongly depends on mineralogy, formation structure, hydrogeology, pH, temperature, pressure, and ionic composition^{87,144}. Reaction rates also vary widely with mineral type: some carbonate reactions may occur relatively quickly, whereas silicate reactions can require much longer periods.

Table 2 summarizes the four principal CO₂ trapping mechanisms in geological storage, together with their main advantages, limitations, and the key parameters that can enhance or reduce their effectiveness.

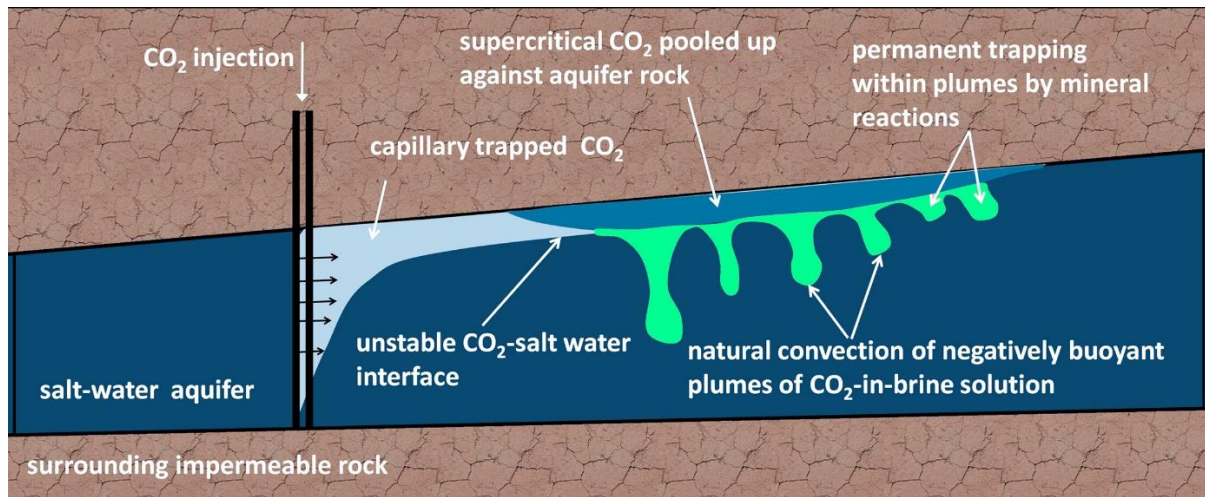


Figure 8. Schematic representation of a typical CO₂ sequestration sequence associated with the evolution of a gravity-driven plume.¹⁴⁵

395 **Table 2.** Summary of the four main CO₂ trapping mechanisms in geological storage.

Trapping mechanism	Main benefits	Main limitations	Factors that may enhance trapping	Factors that may reduce trapping	References
Structural trapping	Provides early containment, serves as the first storage barrier.	Seal damage, spill-point escape, and pressure buildup may threaten containment; monitoring is required.	Strong caprock integrity, secondary sealing layers, suitable injection rate, favorable depth, greater structural closure, CaCO ₃ -rich formation under high injection rate.	Injection pressure above seal entry pressure, leakage pathways, thermal stress in caprock, impurities in injected CO ₂ .	79,104,143,146
Capillary trapping	Restricts plume movement, improves storage efficiency, lowers leakage risk.	Less effective in tight formations; reinjection may become harder with time; trapping can be influenced by resident brine or oil.	Higher flow rate, small-to-medium heterogeneity, more wells, horizontal wells, higher porosity and permeability, denser brine, optimized pressure, CaCO ₃ -rich formation under high injection rate.	Larger grain size, intermediate-wet conditions, drying effects, capillary hysteresis, impurities such as Ar/N ₂ /O ₂ .	79,131,146
Dissolution trapping	Reduces buoyancy, improves storage security, and can increase effective storage through mixing.	Limited by solubility capacity; acidified brine may alter rock and fluid behavior; dissolution may slow after saturation.	Higher flow rate, favorable pressure range, small-to-medium heterogeneity, co-injection of brine and CO ₂ , higher vertical permeability, CaCO ₃ -rich formation under high injection rate.	Higher temperature, higher salinity, higher pH, unfavorable pressure conditions, non-condensable impurities such as Ar/N ₂ /O ₂ .	13,146,147
Mineral trapping	Gives the most permanent storage, converts CO ₂ into an immobile solid, and may further strengthen containment.	Usually develops slowly; depends on reactive minerals and suitable geochemical conditions; precipitation may alter permeability.	Higher pH, abundant Ca ²⁺ , Mg ²⁺ , and Fe ²⁺ , higher pressure, SO ₂ and H ₂ S in injected stream, nucleation sites, ferric-ion-rich host rock.	Low temperature, low pressure, low pH.	34,146,148

2.4 Techniques for Quantifying CO₂ Trapping Mechanisms

2.4.1 Experimental Techniques

Experimental techniques used in geological CO₂ storage research can be divided into three groups: petrophysical analysis, pore-scale experiments, and CO₂-rock-fluid interaction studies⁴⁸. Petrophysical analysis is used to measure bulk reservoir and caprock properties that control CO₂ flow and storage performance. Pore-scale experiments can be used to study microscopic mechanisms of displacement, dissolution, and capillary trapping in porous media. CO₂-rock-fluid interaction studies are used to investigate the chemical and mineralogical changes caused by CO₂ under reservoir conditions. Petrophysical methods commonly include CT scan analysis, high-pressure mercury injection, NMR, conductivity-based measurements, fast resistivity index measurements, automated centrifuge tests, steady-state and pulse-decay permeability tests, standard and dynamic entry-pressure tests, and deuterium tracer techniques¹⁴⁹. At pore scale, typical techniques include micro-CT scanning¹⁵⁰, magnetic resonance imaging (MRI)¹⁵¹, microfluidic experiments¹⁵², and laser fluorescence visualization¹⁵³.

Several researchers have used these methods to investigate the parameters that control trapping and storage performance. For example, Li et al. (2015) used core-flooding and CT imaging to examine capillary trapping of supercritical CO₂ in Berea sandstone. The results showed that 51–75% of the initially injected CO₂ remained trapped after brine injection, and that initial CO₂ saturation had a stronger effect on residual trapping than injection rate¹⁵⁴. At a larger experimental scale, Agartan et al. (2015) investigated the effect of geological heterogeneity on dissolution trapping and mixing behavior in saline formations using two-dimensional tank experiments with different packing configurations. Their results showed that heterogeneity, especially the presence of layered low-permeability zones, can suppress density-driven convective mixing. In homogeneous media, density-driven fingering enhanced downward transport and promoted greater contact between dissolved CO₂ and the formation¹⁵⁵.

Other studies have focused on the role of geochemical reactions in altering storage behavior. Rathnaweera et al. (2016) investigated how long-term exposure to brine and supercritical CO₂ alters the properties of sandstone samples. In their study, sandstone was aged 1.5 years under brine and supercritical CO₂ conditions. The results showed a significant decrease in pH due to brine acidification caused by dissolved CO₂. This occurred because CO₂ dissolution released free H⁺ ions into the brine, which promoted mineral dissolution and altered

the mineralogical composition of the sandstone. The authors concluded that these geochemical alterations could modify the rock structure and potentially affect permeability¹⁵⁶. Similarly, experiments on Bentheimer sandstone suggested that brine salinity has a strong influence on storage performance and that an optimal salinity range may exist for CO₂ storage¹⁵⁷. More recently, Mathew et al. (2026) showed that CO₂ solubility increased with pressure but decreased with higher temperature and brine salinity¹⁵⁸.

Another important study has examined injectivity impairment and formation damage during CO₂ injection. Yusof et al. (2022) experimentally investigated injectivity impairment caused by the combined effects of salt precipitation and fines migration during CO₂ injection. Their results showed a clear direct relationship between brine salinity and injectivity reduction, with higher salinity leading to higher reduction in permeability. The study also found that fines migration further escalated injectivity impairment. To represent migrating fines, the authors used nanoparticles of different sizes, allowing them to evaluate how particle size influenced the severity of formation damage¹⁵⁹. This behavior is commonly explained by the dry-out effect, which increases the precipitation of NaCl particles near the wellbore and consequently reduces porosity and permeability. When supercritical CO₂ is injected into the reservoir, evaporation of water into the CO₂-rich phase increases the salinity of the remaining brine. As this process continues, the salt concentration may exceed the NaCl solubility limit at the current pressure and temperature conditions¹⁶⁰. As a result, salt precipitates and blocks pores.

Overall, the experimental literature shows that CO₂ trapping, and storage performance are controlled by a broad set of coupled factors, including initial CO₂ saturation, geological heterogeneity, mineral reactions, salinity, wettability, and near-wellbore salt precipitation. Core-scale and pore-scale studies have therefore been essential for identifying the mechanisms through which these parameters influence injectivity, migration, residual trapping, dissolution trapping, and long-term containment. However, because such experiments are usually performed on limited spatial and temporal scales, their ability to fully characterize field-scale and long-term processes remains restricted.

2.4.2 Numerical and Simulation-Based Techniques

Numerical modeling is often used to quantify trapping indices in deep saline aquifers, particularly those related to residual, solubility, and mineral trapping. Early numerical study by Ide et al. (2007) focused on residual trapping. The authors examined how gravity, viscous, and capillary forces control capillary trapping. Their results showed that weaker gravitational

forces relative to viscous forces led to greater residual trapping, whereas stronger gravity reduced the trapped fraction. They also demonstrated that capillary pressure, aquifer dip, and injection strategy, such as alternating CO₂-brine injection or post-CO₂ brine injection, can further enhance residual trapping efficiency ¹²⁹.

Subsequent studies extended the analysis to thermodynamic controls on dissolution trapping. For example, Pasdar et al. (2015) evaluated the influence of pressure, temperature, and salinity on CO₂ storage in saline aquifers and found that salinity exerted the strongest control on CO₂ dissolution compared with temperature and pressure ¹⁶¹. A similar conclusion was later reported by Kinate et al. (2024), who showed that higher brine salinity reduces CO₂ dissolution and improves larger gas-cap development, which shifts storage behavior away from dissolution trapping toward greater free-phase accumulation ¹⁶². Tabrizinejadas et al. (2023) demonstrated that temperature also plays an important role in dissolution processes. Their field-scale numerical model showed that temperature effects increase fingering and enhance CO₂ dissolution, whereas neglecting thermal convection can significantly alter predictions of CO₂ transport and dissolution behavior ¹⁶³.

In parallel, several numerical studies have emphasized the importance of wettability as a major factor that affects plume migration and trapping. Khedheawi et al. (2016) showed that rock wettability strongly affects CO₂ migration and trapping in deep saline aquifers: water-wet rocks improved residual trapping, whereas CO₂-wet rocks allowed farther upward plume migration and more efficient solubility trapping ¹⁶⁴. More recently, Khoramian et al. (2025) expanded this work by the combination of wettability, salinity, and temperature within a reactive transport framework. Their results showed that elevated temperature promotes CO₂ mineralization but reduces capillary trapping and increases dissolution trapping. They further demonstrated that wettability itself demonstrates a dominant control on both multiphase distribution and geochemical reactions. They showed that CO₂-wet conditions are more favorable for stronger dissolution and mineral trapping, whereas strongly water-wet conditions improve capillary and residual trapping ^{40–42}.

Another major direction in numerical research has been the role of heterogeneity in plume shape and storage efficiency. Sohal et al. (2021) showed that stronger permeability contrasts in fractured carbonate systems can enhance CO₂ retention ⁴⁴. This was further extended by Wang et al. (2024), who investigated permeability heterogeneity in deep saline aquifers using an SGSIM-based heterogeneous model with different horizontal and vertical correlation lengths. They classified plume behavior into dispersive, fingering, channeling, and

sweeping flow patterns and showed that storage efficiency peaks when the horizontal and vertical correlation lengths are around 0.1–0.2, as this configuration increases the safely trapped fraction and delays breakthrough¹⁶⁵.

Numerical studies have also been used to investigate long-term mineralization trapping. For instance, Bello et al. (2024) conducted a sensitivity analysis of mineralization trapping in a deep saline aquifer by varying injection period, pressure, temperature, salinity, and mineral composition. Their simulations showed that mineral trapping is a slow process, contributing only about 8.9% of total trapped CO₂ after 100 years, but increasing to 76% after 1000 years¹⁶⁶. They also found that longer injection periods enhance mineralization efficiency and that mineral reactions depend strongly on mineral composition and temperature, with calcite and dolomite favored at low to medium temperatures and quartz, K-feldspar, kaolinite, and illite favored at higher temperatures¹⁶⁶.

Salt precipitation has also been investigated numerically at the field scale. For example, Papi et al. (2025) used the CMG-GEM simulator to evaluate methods for preventing salt precipitation during CO₂ storage in saline aquifers. Their results showed that dissolved-water CO₂ injection can substantially reduce salt precipitation by limiting further water evaporation into the CO₂-rich phase. Fully water-saturated CO₂ reduced salt precipitation nearly to zero, while dissolving 2000 ppmv water in the injected CO₂ decreased precipitation to about one-third of the conventional case. These findings suggest that humid or dissolved-water CO₂ injection could be an effective strategy for mitigating injectivity loss and pressure buildup caused by salt precipitation near the wellbore¹⁶⁷.

Overall, these numerical studies show that trapping efficiency in deep saline aquifers is governed by a complex interplay of flow forces, thermodynamic conditions, wettability, heterogeneity, geochemical reactions, and operational effects. Together, they provide important insight into how different mechanisms dominate over different spatial and temporal scales, and they demonstrate the value of numerical modeling for predicting both short-term storage performance and long-term trapping security.

2.4.3 Machine Learning-Based Techniques

Although physics-based reservoir simulators are widely used to quantify CO₂ trapping efficiency, their application in broad parametric screening is often limited by the high computational cost of running long-term, high-resolution models. This limitation has accelerated interest in ML surrogates for estimating trapping indices. Baghban et al. (2017) developed a least-squares support vector machine (LSSVM) model to estimate the solubility

trapping index in saline aquifers using reservoir pressure and temperature variables, solution composition descriptors, and molecular weight¹⁶⁸. Jeong et al. (2018) assessed neural network models and support vector regression for predicting CO₂ storage performance in saline formations¹⁶⁹. Beyond these individual studies, multiple studies have trained ML algorithms on simulation datasets - often compiled from the literature - to predict residual (RTI) and solubility (STI) trapping indices across a range of reservoir conditions.^{45,170,171} Safaei-Farouji et al. further extended this direction by evaluating ensemble learners and neuro-fuzzy approaches for trapping prediction over broad operational and reservoir parameter spaces¹⁷².

Khanal & Shahriar (2022) extended ML-based prediction frameworks to include mineral trapping index (MTI) alongside residual and solubility trapping, demonstrating high predictive accuracy using tree-based and boosting algorithms¹⁷³. Cheng et al. (2025) developed an ML framework for predicting multiphase CO₂ trapping in deep saline aquifers and combined it with an inverse design workflow to identify operating conditions that maximize mineral trapping. Their results also showed that depth and permeability are the dominant controls on dissolved, residual, and mineral trapping¹⁷⁴. Tariq et al. (2025) developed a machine-learning framework to rapidly predict safe CO₂ trapping indices based on long-term reservoir simulations⁴⁶. Their workflow accounts for reservoir heterogeneity, cap-rock behavior, coupled multiphase flow, geochemistry, and geomechanics, and they then used these simulation results to train several ML models. The best performance was achieved by a fully connected neural network, reproducing long-term trapping indices. More recently, Davoodi et al. (2025) developed an optimized deep-learning framework to predict subsurface CO₂ trapping efficiency, focusing on both residual trapping index (RTI) and solubility trapping index (STI). Using 6811 data points, they combined CNN and LSTM models with optimization algorithms and feature-selection methods and found that the hybrid optimized models outperformed standard deep-learning approaches. In particular, the CNN-COA model achieved the best accuracy, while SHAP analysis identified residual gas saturation, permeability, salinity, thickness, and porosity as the most influential inputs¹⁷⁵. Beyond identifying influential variables, recent work has also demonstrated the feasibility of embedding physical knowledge directly into data-driven models. For example, Vo Thanh (2026) incorporated key physical factors such as Henry's law, the Setchenow effect, and gas compressibility into a physics-informed ML framework for predicting hydrogen solubility, improving both predictive accuracy and consistency with governing laws¹⁷⁶.

Table 3 summarizes prior studies that used ML models to predict CO₂ trapping indices in saline aquifers. Previous studies have provided valuable insights into CO₂ trapping behavior and have significantly advanced the understanding of storage mechanisms. Despite this progress, most existing ML-based GCS studies rely on dimensional reservoir and operational parameters as direct model inputs and do not explicitly incorporate dimensionless groups that encode the governing physics of CO₂ migration and trapping. Although variables such as permeability, porosity, thickness, depth, and injection conditions are important for the description of a reservoir, their direct use often makes predictive models strongly dependent on the specific ranges represented in the training dataset. As a result, such models may become less transferable across different reservoirs conditions. In addition, the relationship between individual dimensional variables and trapping performance is often indirect. For example, depth does not control trapping independently, but influences pressure, density contrast, buoyancy, and gravity segregation, which then affect plume migration, mixing, dissolution, and trapping. Similarly, permeability and porosity do not govern trapping alone, but through their interaction with viscous, capillary, and gravitational forces. Therefore, models based only on dimensional variables may be less interpretable, because it is difficult to directly relate a single raw parameter to the trapping mechanisms.

This limitation motivates the use of a physics-guided formulation based on dimensionless groups. Related studies in CO₂-EOR and CO₂ storage have shown that predictive equations based on dimensionless numbers can provide a more compact and physically meaningful representation of subsurface performance. For example, Algharaib and Alajmi (2025) expressed oil recovery factor and CO₂ storage capacity as functions of four dimensionless numbers and demonstrated that storage-related performance can be represented through grouped variables rather than a large set of separate dimensional inputs¹⁷⁷. Likewise, Li et al. (2015) used a reduced-order framework to evaluate CO₂-EOR and storage performance over a wide range of reservoir heterogeneities and fluid properties, which shows the value of physically guided grouped inputs for broader parametric prediction¹⁷⁸. Compared with raw dimensional parameters, dimensionless groups reduce the number of inputs, lessen dependence on variable-specific ranges, and improve interpretability, which connects the model inputs more directly to the balance of forces controlling flow and trapping. Accordingly, this thesis develops a physics-guided ML framework in which the input variables are expressed as dimensionless groups to predict all three trapping indices. In this work, the aim is to build a

592 computationally efficient and more transferable predictive framework that better reflects the
593 governing physics of CO₂ migration and trapping. Additionally, it creates a tool for rapid
594 scenario evaluation and sensitivity analysis in deep saline aquifers.

Table 3. Summary of ML models used to predict different trapping mechanisms

Year	Input parameters and ranges	Output parameters	Models used	Best model (Test metrics)	Reference
2020	Depth (800–2000 m), permeability (10–200 mD), permeability aspect ratio kh/kv (0.001–0.1), porosity (0.10–0.30), salinity (10–300 kppm), residual gas saturation Sgr (0.20–0.50), and thickness (10–200 m)	RTI, STI, and TEI	ANN	ANN $R^2 \approx 0.9847$ / $RMSE \approx 0.0082$	37
2022	Depth (800–3000 m), permeability (0.01–2000 mD), permeability aspect ratio Kv/Kh (100–1500), porosity (0.01–0.40), salinity (10,000–400,000 ppm), residual gas saturation (0.10–0.50), thickness (2–200 m), CO ₂ injection rate (39–5480 ton/day)	RTI, STI, and TEI	GPR, SVM, and RF	GPR RTI: $R^2 = 0.9982$; $RMSE = 0.005$, STI: $R^2 = 0.9953$; $RMSE = 0.009$, TEI: $R^2 = 0.9953$; $RMSE = 0.009$	170
2022	Absolute permeability (5.6–2029 mD), net thickness (5–1500 m), reservoir depth (704.69–3853 m), reservoir temperature (30°C–73°C), Porosity (10^{-4} –0.47), injection rate (2.8–68,573 ton/day), elapsed time (8–9185 years).	RTI, STI	ANFIS, ET, RF, and RBF networks.	RF RTI: $R^2 = 0.995$ $RMSE = 0.0073$, STI: $R^2 = 0.965$, $RMSE = 0.0086$	172
2022	Injection period (3.8–100 years), post-injection period (7.65–7988 years), porosity (0.093–0.47), permeability (5.6–2029 mD), thickness (5–1500 m), salinity (10,000–320,000 ppm), depth (705–3853 m), residual gas saturation Sgr (0–0.5), injection rate (3.47–65,753 ton/day).	RTI, STI	SVR, RF, and XGBoost	XGBoost RTI: $R^2 \approx 0.9916$ and $RMSE \approx 0.0241$ STI: $R^2 \approx 0.9941$ and $RMSE \approx 0.0134$	45
2022	Grid thickness (2.5–10 m), gas residual saturation (0.1–0.5), gas injection rate (5000–15,000 m ³ /day), permeability log value (0–3.69897), kv/kh (1–10), porosity (0.08–0.40), simulation time (5–300 years).	RTI, STI, and MTI	MLP, RF, SVR, and XGBoost	XGBoost RTI: $R^2 = 0.99988$, $RMSE = 0.08690$, STI: $R^2 = 0.99985$, $RMSE = 0.07781$ MTI:	173

$R^2 = 0.99968$, $RMSE = 0.07606$

2025	Dykstra–Parsons coefficient VDP (0.167–0.938), average porosity (0.062–0.394), injection rate (0–5 m ³ /day), Biot’s coefficient (0.6–0.9), Young’s modulus (5.1–50 GPa), Poisson’s ratio (0.2–0.4), perforation thickness (3.66–120 m), reservoir thickness (20–200 m), salinity (1000–100000 ppm), temperature (60°C–110°C), time (0.1–200 years)	Structural trapping index, RTI, STI, and MTI	ANN, DT, RF, K-KNN, XGBoost, and AdaBoost	ANN StTI: $R^2 = 0.991$, $RMSE = 1.86 \times 10^{-2}$ RTI: $R^2 = 0.990$, $RMSE = 1.41 \times 10^{-2}$ STI: $R^2 = 0.995$, $RMSE = 1.51 \times 10^{-2}$ MTI: $R^2 = 0.998$, $RMSE = 7.0 \times 10^{-4}$	46
2025	Porosity (Por): 0.0001–0.470 fraction; Permeability (Perm): 5.60–2029 mD; Thickness (Th): 0.50–1500 ft; Salinity (Sal): 0–320000 ppm; Depth: 704–3853 ft; Residual gas saturation (RGS): 0.05–0.50 fraction; Injection rate (IR): 2.80–65753 MSCF/D; Elapsed time (Te): 8–10000 days	RTI, STI	CNN, LSTM, hybrid deep-learning models combined with growth optimization (GO) and cuckoo optimization algorithm (COA)	CNN–COA. RTI: $R^2 = 0.99997$, $RMSE = 0.0035$; STI: $R^2 = 0.9994$, $RMSE = 0.0028$	175
2025	Porosity: 0.20–0.35; Permeability: 500–2000 mD; Depth: 1000–2500 m; Injection rate: 5000–20000 m ³ /day; Maximum gas saturation: 0.40–0.60; Temperature gradient: 25–30 °C/km	RTI, STI, and MTI	TabTransformerLite, SAINTLite, NODELite, linear models, SVR, tree ensemble models, ANN	TabTransformerLite nRMSE = 0.033, $R^2 = 0.92$	174

Root Mean Squared Error (RMSE)

Coefficient of Determination (R^2)

3. METHODOLOGY

This section outlines the methodological workflow used to construct the simulation dataset, including the governing formulation, reservoir model setup, initial and boundary conditions, and parameter ranges. A commercial compositional simulator (CMG-GEM)¹⁷⁹ was employed to generate the multiphase flow outputs required to quantify CO₂ trapping mechanisms.

3.1 Governing Equation

The governing mass-balance equation (**Equation (1)**) describes multiphase, multicomponent flow by accounting for four main contributions: (i) the temporal change in fluid accumulation, (ii) advective movement driven by pressure and gravity, (iii) chemical reactions affecting component mass, and (iv) source–sink terms associated with well injection or production.

$$\begin{aligned} \frac{\partial}{\partial t} \left(\phi \sum_{\alpha} S_{\alpha} \rho_{\alpha} x_{\alpha i} \right) - \nabla \cdot \left\{ K \sum_{\alpha} \frac{k_{r\alpha}}{\mu_{\alpha}} \rho_{\alpha} x_{\alpha i} (\nabla p_{\alpha} + \rho_{\alpha} g \nabla Z) \right\} + r_i \\ + \sum_l \left(\sum_{\alpha} \rho_{\alpha} x_{\alpha i} q_{\alpha}^l \right) = 0 \end{aligned} \quad (1)$$

In the above formulation, ϕ is porosity and t denotes time. S_{α} and ρ_{α} are the saturation and density of phase α , respectively, and $x_{\alpha i}$ is the mole fraction of component i in phase α . The absolute permeability is given by k , while $k_{r\alpha}$ and μ_{α} represent the relative permeability and viscosity of phase α . The pressure of phase α is p_{α} ; g is the gravitational acceleration and Z is depth. The term q_{α} denotes the well source or sink rate (volumetric injection or production) for phase α . Here, i indexes the chemical components (CO₂ and H₂O), and α indicates the coexisting phases, including supercritical CO₂ and the aqueous brine phase.

3.2 Trapping indices

Trapping mechanisms in geological CO₂ storage are commonly described using three main components: residual, solubility, and mineral trapping.³⁶ In this study, the supercritical CO₂ index (SCI) represents the fraction of injected CO₂ that remains in the supercritical phase, i.e., the portion that is not dissolved in brine and is not converted into solid minerals. The

residual trapping index (RTI) quantifies CO₂ immobilized by capillary forces. The solubility trapping index (STI) accounts for CO₂ dissolved in formation brine, whereas the mineral trapping index (MTI) measures mineralized amount of CO₂. Together these indices provide a quantitative basis for assessing storage performance. Definitions are provided in **Equations (2) – (5)**:

$$SCI = \frac{\text{Total CO}_2 \text{ in Supercritical state (moles)}}{\text{Total injected CO}_2 \text{ (moles)}} \times 100\% \quad (2)$$

$$STI = \frac{\text{Total CO}_2 \text{ Dissolved (moles)}}{\text{Total injected CO}_2 \text{ (moles)}} \times 100\% \quad (3)$$

$$RTI = \frac{\text{Total CO}_2 \text{ residually trapped (moles)}}{\text{Total injected CO}_2 \text{ (moles)}} \times 100\% \quad (4)$$

$$MTI = \frac{\text{Total CO}_2 \text{ mineralized (moles)}}{\text{Total injected CO}_2 \text{ (moles)}} \times 100\% \quad (5)$$

3.3. Model description

For training the ML models, a dataset is required. For this purpose, a reservoir model was constructed using a traditional numerical simulator. This model was further used to generate a large long-term (200-year) dataset. The main operational and reservoir parameters were pre-sampled, after which multiple simulation runs were performed. The model description, as well as a detailed description of the dataset generation and ML training process, are provided below.

3.3.1 Aquifer configuration

The models consist of a three-dimensional radial grid (150 × 1 × 25) extending to a 1 km radius. The well is perforated in the bottom three layers. The grid and boundary conditions are fixed, while reservoir initial reservoir pressure, reservoir temperature, brine salinity, vertical-to-horizontal permeability ratio (k_v/k_h), residual gas saturation (S_{gr}), carbon dioxide injection rate, and reservoir thickness varied treated as variables. Geological heterogeneity was parameterized via mean permeability, porosity, and the Dykstra–Parsons coefficient.

The simulated fluid system comprised two components: water (as brine) and CO₂. The phase interactions were modeled using the Peng–Robinson equation of state.¹⁸⁰ Thermophysical data were sourced from CMG’s fluid property libraries, and CO₂ solubility in brine was dynamically updated during simulations based on pressure, temperature, and salinity changes. No-flow (closed) boundary conditions were applied at the top, bottom, and lateral edges of the domain to mimic natural confinement, effectively simulating impermeable barriers formed by surrounding geological formations.¹⁸¹ CO₂ was injected vertically at a constant rate through a well perforated in last three layers. Each simulation included 1 year of injection, followed by 199 years of monitoring the post-injection migration of the CO₂ plume. **Figure 9** shows a schematic of the base model cross-section.

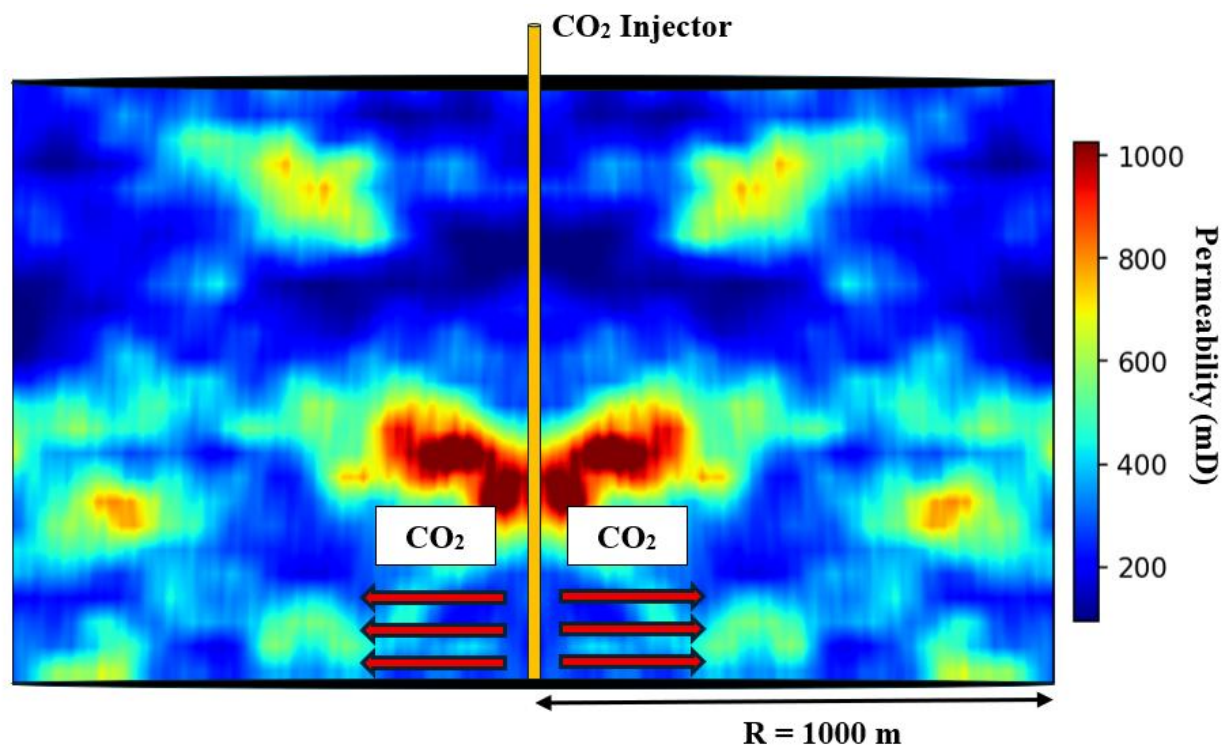


Figure 9. Base case model radial cross-section of the aquifer model showing the 1-km radial extent, vertical thickness, and spatial permeability variability.

3.3.2 Wettability settings

In our GCS simulations, the saline aquifer is initially saturated with brine, after which supercritical CO₂ is injected. To represent the resulting two-phase flow, relative-permeability and capillary pressure functions for the aqueous and CO₂ phases are required, since they control the effective permeability and phase distribution. In this study, both the relative permeability

and capillary pressure are described using the Brooks–Corey correlation¹⁸², given by
Equations (6)–(9):

$$k_{rw} = (S_w^*)^{\frac{2+3\lambda}{2\lambda}} \quad (6)$$

$$k_{rg} = (1 - S_w^*)^{0.5} \left[1 - (S_w^*)^{\frac{1+\lambda}{\lambda}} \right]^2 \quad (7)$$

$$S_w^* = \frac{S_w - S_{wir}}{1 - S_{wir} - S_{gc}} \quad (8)$$

$$P_c = P_e \left((S_w^*)^{-1/\lambda} - 1 \right) \quad (9)$$

where the symbol λ represents the pore-size distribution index; k_{rw} refers to the relative permeability of the brine phase, k_{rg} denotes the relative permeability of the supercritical CO₂ phase, and S_w^* denotes the effective water saturation. Figure 2 shows the relative permeability and capillary pressure curves. **Figure 10**

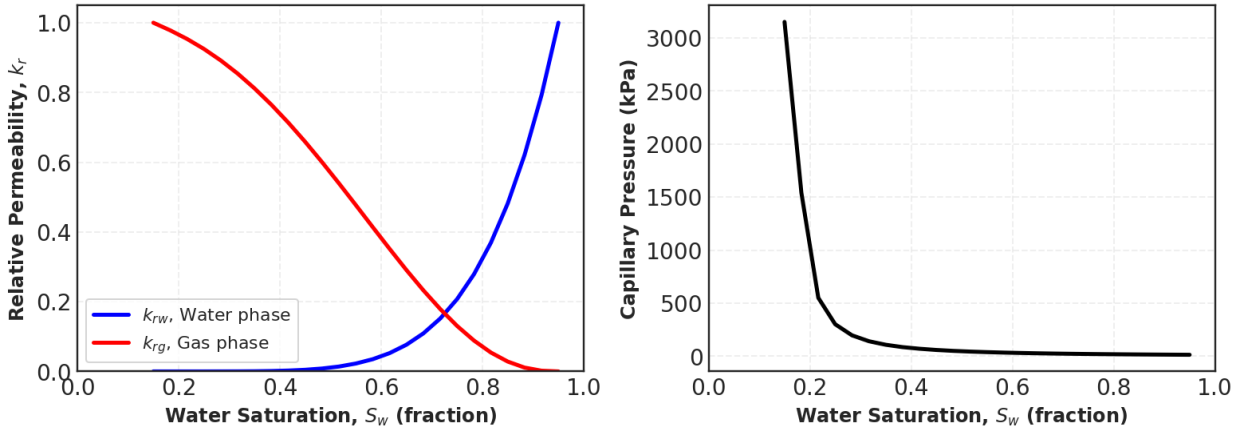


Figure 10. Relative permeability and capillary pressure used in this study

3.3.3 Geochemical Reactive Transport Modeling

The geochemical model used in this study represents a carbonate reservoir system, and the mineralogical composition, mineral fractions, and CMG-GEM implementation details were adopted directly from our previously published work⁴² to ensure full consistency with the established carbonate characterization and reaction framework.

3.3.3.1 Intra-aqueous reactions

The intra-aqueous chemistry considered in this work describes the dissolution of CO₂ into the aqueous phase and the subsequent speciation of carbonate ions.¹⁸³ The dominant processes are captured through the equilibrium reactions listed in **Equations (10)–(13)**:



These reactions are treated as equilibrium processes rather than kinetically controlled reactions. This assumption is justified because intra-aqueous reactions typically occur on very short timescales, ranging from milliseconds to seconds, when compared with the much longer characteristic times of fluid migration and mineral reaction fronts, which span hours to years.^{184–186} Owing to their rapid and reversible behavior, the aqueous reactions are therefore assumed to adjust quasi-instantaneously to local variations in pH, ionic strength, and dissolved CO₂ concentration.

3.3.3.2 Mineral reactions

Mineral reactions were represented in the reactive transport simulations using kinetic rate laws derived from Transition State Theory (TST)¹⁸⁷ and implemented in CMG-GEM via the process wizard. The mineral reaction rate r_β describes the kinetic behavior governing mineral dissolution and precipitation, as expressed in **Equation (14)**.

$$r_\beta = A_\beta k_\beta \left(1 - \frac{Q_\beta}{k_{\text{eq}}} \right) \quad (14)$$

The reactive surface area A is continuously updated throughout the simulation according to **Equation (15)**:

$$A = \bar{A}_0 \frac{N_m}{N_{m0}} \quad (15)$$

where A and $\bar{A}_0$ represent the reactive surface areas at the current and initial times, respectively, and N_m and N_{m0} denote the mineral moles at the current and initial times, respectively.

The saturation index (SI) is defined as the ratio Q_β/k_{eq} . The SI value controls the direction of mineral reactivity: a positive SI corresponds to precipitation, whereas a negative SI corresponds to dissolution. The rate constant k_β , which controls the reaction rate at the current temperature T , is evaluated using the Arrhenius rate constant expression given in **Equation (16)**:

$$k_\beta = k_{0\beta} \exp \left[-\frac{E_{a\beta}}{R} \left(\frac{1}{T} - \frac{1}{T_0} \right) \right] \quad (16)$$

where $k_{0\beta}$ is the reaction rate at the reference temperature, $E_{a\beta}$ is the activation energy in J/mol, R is the universal gas constant, T is the current temperature, and T_0 is the initial temperature.

The main reactive minerals in the system are calcite, kaolinite, anorthite, and halite. Among these, anorthite dissolution is particularly important, as it supplies Ca^{2+} , Al^{3+} , and H_4SiO_4 that support both secondary carbonate precipitation and kaolinite formation, thereby linking feldspar reactivity to the aquifer's long-term mineral trapping capacity. Together, these reactions capture the geochemical feedback induced by CO_2 injection, including acid-driven primary mineral dissolution and the subsequent secondary phase formation. In contrast to fast aqueous speciation, mineral reactions evolve on longer timescales and must therefore be treated with time-dependent kinetics. Geochemical reactions^{188,189} and their corresponding parameters are shown in **Table 4**.

Table 4. Mineral reactions defined by the geochemical model

Reaction	Log $K_{eq,m}$	TST rate constant (mol/m ² s)	Reactive surface area (m ² /m ³)	Activation energy (J/mol)
$\text{CaAl}_2\text{Si}_2\text{O}_8 + 8\text{H}^+ \rightarrow 2\text{SiO}_2 + 2\text{Al}^{3+} + \text{Ca}^{2+} + 4\text{H}_2\text{O}$	31.75	-9.12	2760.29	17800
$\text{CaCO}_3 + \text{H}^+ \rightarrow \text{Ca}^{2+} + \text{HCO}_3^-$	2.07	-5.81	2709.95	23500
$\text{Al}_2\text{Si}_2\text{O}_5(\text{OH})_4 + 6\text{H}^+ \rightarrow 2\text{SiO}_2 + 2\text{Al}^{3+} + 5\text{H}_2\text{O}$	9.73	-13.1798	2594.05	22200
$\text{NaCl} \rightarrow \text{Na}^+ + \text{Cl}^-$	0.21	-0.21	2163.35	7400

3.4 Generation and analysis of datasets

3.4.1 Sample parameters

A set of reservoirs, operational, and heterogeneity-controlling parameters, along with their corresponding ranges, was defined and systematically sampled to create the dataset. The uncertain parameters include initial reservoir pressure, reservoir temperature, brine salinity, vertical-to-horizontal permeability ratio (k_v/k_h), residual gas saturation (S_{gr}), carbon dioxide injection rate, and reservoir thickness. In addition, three parameters controlling geostatistical heterogeneity were treated as uncertain: mean permeability, mean porosity, and the Dykstra–Parsons coefficient (V_{DP}), which governs the degree of permeability variability. Uncertainty analysis and parameter sampling were implemented in CMG-CMOST, where all uncertain parameters were sampled using a Latin hypercube sampling (LHS) design to efficiently explore the multidimensional parameter space and generate diverse scenarios. The parameter ranges were selected based on previous studies^{45,173,190} and are summarized in **Table 5**.

Table 5. Ranges of CMOST input parameters used for dataset generation and uncertainty analysis.

Parameter	Units	Min	Max
Reservoir thickness	m	125	250
Initial reservoir pressure (IRP)	MPa	8	15
Reservoir temperature	°C	40	70
Brine salinity	M	0.173	5.13
Vertical to horizontal permeability ratio	-	0.1	1
Residual gas saturation (RGS)	-	0.1	0.5
CO ₂ injection rate	m ³ /day	200000	800000
Mean permeability	mD	200	1000
Mean porosity	frac.	0.05	0.4
Dykstra–Parsons coefficient	-	0.1	0.9

3.4.2 Heterogeneity Modeling

We generated permeability and porosity heterogeneity using a geostatistical Matérn-based spatial random field generator implemented in the open-source GStools Python library¹⁹¹. A two-dimensional anisotropic Matérn covariance model¹⁹² was defined in the radial–vertical plane, with separate correlation lengths in the radial and vertical directions to reproduce realistic stratified heterogeneity patterns. A structured random field realization for

each case was sampled on the simulation grid and mapped to permeability using the target mean permeability and the Dykstra–Parsons coefficient (V_{DP}).

Mean permeability, VDP, and target mean porosity were treated as uncertain inputs and sampled jointly with other model parameters using a Latin hypercube sampling (LHS) design¹⁹³. Permeability was generated independently of porosity to preserve the prescribed heterogeneity structure. The permeability field was subsequently used to derive porosity by inverting the Kozeny–Carman relationship¹⁹⁴, with the Kozeny–Carman constant calibrated such that the resulting porosity field matches the sampled mean porosity. A small stochastic perturbation was added to the porosity field to represent the natural variability in the porosity–permeability relationship⁴². After the permeability field was generated, VDP was recalculated using **Equation (17)**. The resulting permeability and porosity fields were exported as CMG–GEM include files and assigned to the simulation grid for each heterogeneity scenario. Figure 3 shows a randomly selected example of permeability and porosity fields.

$$V_{DP} = \frac{k_{50} - k_{84.1}}{k_{50}} \quad (17)$$

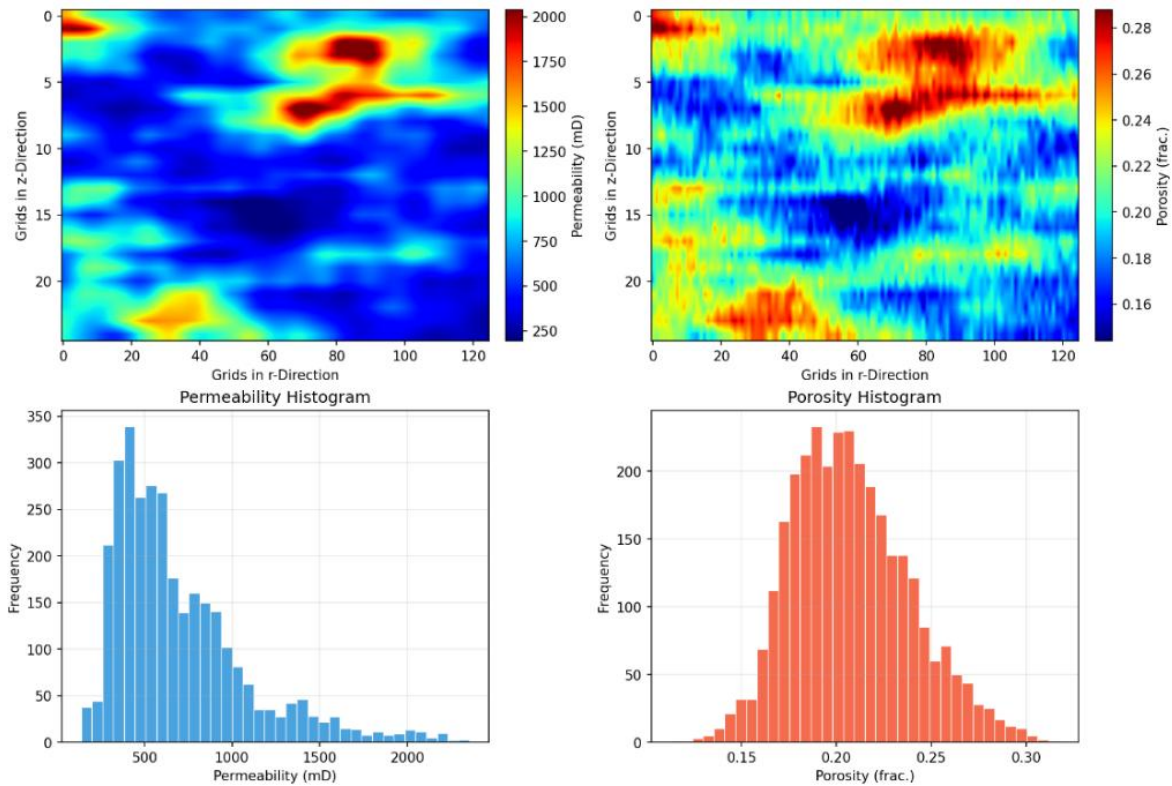


Figure 11. Permeability and porosity fields with corresponding histograms ($V_{DP} = 0.677$, mean $K = 692.5$ mD, mean $\phi = 0.213$)

3.4.3 Construction of feature set

The raw sampled inputs were transformed into physically motivated dimensionless features to improve model transferability and reduce sensitivity to absolute units. Dimensionless features are designed to encode the dominant physical mechanisms that control CO₂ plume migration and trapping in saline aquifers.

The dimensionless gravity number ¹⁷⁷ defined in **Equation (18)** was used to characterize the competition between buoyancy forces and viscous forcing during injection. High gravity corresponds to greater gravity force, causing the CO₂ plume to segregate more vertically and reduce lateral sweep efficiency. In contrast, lower gravity numbers indicate that viscous forces are more dominant, allowing the plume to spread more broadly across the reservoir. This wider distribution increases the contact area between gas and brine:

$$G = 8.473 \times 10^{-7} \left(\frac{k_v}{k_h} \right) \times k_{mean} \times A \times \frac{\rho_w - \rho_g}{q * \mu_g} \quad (18)$$

where k_v/k_h is the vertical-to-horizontal permeability ratio (–), k_{mean} is the mean permeability (mD), and A is the cross-sectional area perpendicular to the dominant flow direction (m²). The terms ρ_w and ρ_g denote brine and gas densities (kg/m³), respectively, μ_g is the gas viscosity (cP), and q is CO₂ injection rate (m³/day). The constant 8.473×10^{-7} is a unit conversion factor.

The injected pore volume, defined in **Equation (19)**, represents the amount of injected CO₂ relative to the reservoir's storage capacity, which is affected by both porosity and reservoir thickness. As injected pore volume increases, the CO₂ plume spreads through reservoir and remains in contact with the brine for longer time. This extended interaction not only improves solubility trapping but also creates more favorable conditions for long-term mineralization to occur.

$$Q_d = \frac{q \times 365}{PV} \quad (19)$$

where q is the injection rate (m³/day) and PV is the reservoir pore volume (m³).

The dimensionless pressure drawdown, as defined in **Equation (20)**, represents how strong the applied injection pressure is compared to the reservoir's original pressure state. Higher drawdown values indicate greater viscous resistance to flow, which directly impacts how easily CO₂ can be injected, how it moves through the reservoir, and how it's divided between mobile phases and residually trapped gas:

$$D_d = \frac{WBHP - p_{ref}}{p_{ref}} \quad (20)$$

where WBHP is the wellbore bottom-hole pressure (kPa) and p_{ref} is the initial reservoir pressure (kPa).

The final set of engineered features used to train the machine learning models includes injected pore volume, dimensionless pressure drawdown, gravity number, temperature, salinity, and the Dykstra–Parsons coefficient. This selection captures the key physical factors that govern CO₂ movement and trapping.

3.4.4 Data analytics

Once the simulations and feature construction were completed, all the data were combined into a single dataset for building the machine learning models. In total, 523 simulation cases were run using CMG-GEM and CMOST, with each case producing output at 64 different time steps - annually from year 1 to 30, and then every five years from year 30 up to 200. From these raw simulation results, the previously defined dimensionless features were calculated. This finalized dataset forms the foundation for training, validating, and testing the machine learning models in the next stages of the study.

A descriptive statistical analysis was performed on both the input parameters and model outputs to characterize the dataset. This analysis included metrics such as standard deviation, variance, kurtosis, skewness, overall range, upper and lower bounds, and interquartile ranges at the 25th, 50th, and 75th percentiles. These statistics help reveal the variability, spread, and overall distribution of the data, confirming that the dataset effectively captures the intended uncertainty space. The wide range of values across different variables shows that the simulations span multiple physical regimes, including both gravity- and viscous-dominated conditions. Additionally, the lack of strong clustering and the presence of well-balanced interquartile ranges suggest that the dataset is not overly concentrated in a narrow set of physical conditions. Also, the distinct statistical spreads of the trapping indices reflect their physical behavior. **Table 6** presents a summary of these statistical measures.

Table 6. Descriptive statistics of the generated dataset used for developing the machine-learning model.

Parameter	mean	standard deviation	variance	kurtosis	skewness	lower bound	25 percent	50 percent	75 percent	upper bound
PV injected (-)	1.834	1.497	2.241	6.935	2.310	0.292	0.880	1.339	2.290	10.733
Dimensionless drawdown (-)	0.462	0.291	0.085	8.843	2.349	0.110	0.265	0.386	0.569	3.238
V _{DP} (-)	0.501	0.231	0.053	-1.197	-0.003	0.100	0.300	0.501	0.701	0.900
Reservoir temperature (°C)	55.028	8.661	75.022	-1.199	0.000	40.000	47.514	55.029	62.543	70.000
Salinity (M)	2.651	1.435	2.059	-1.203	0.001	0.173	1.405	2.647	3.898	5.130
Residual gas saturation ()	0.300	0.116	0.013	-1.198	-0.002	0.100	0.200	0.300	0.401	0.500
Gravity Number ()	0.278	0.320	0.103	14.629	3.177	0.007	0.088	0.169	0.338	2.615
Elapsed time (years)	69.688	62.485	3904.394	-0.999	0.661	1.000	16.750	42.500	121.250	200.000
Supercritical CO ₂ concentration (%)	59.611	14.866	221.003	-0.303	-0.593	13.491	50.012	61.972	71.230	92.061
Dissolved CO ₂ (%)	30.753	9.966	99.326	-0.685	0.359	7.234	22.843	29.515	37.929	58.564
Residually trapped CO ₂ (%)	51.099	13.346	178.118	-0.483	-0.295	11.948	41.605	51.970	61.134	81.123
Mineralized CO ₂ (%)	2.256	1.914	3.664	2.382	1.127	1.713	1.011	2.035	3.097	14.687

3.5 Machine learning techniques

This study employed different supervised machine-learning techniques to predict CO₂ trapping indices, including linear regression (LR), decision tree (DT), random forest (RF), XGBoost (XGB), LightGBM, CatBoost, FT-Transformer, TabM, and symbolic regression (SR).

Linear regression (LR) is one of the most widely used statistical learning methods for modeling the relationship between input variables and a continuous target. It assumes that the target variable can be expressed as a linear combination of the input variables and estimates

the model weights. It minimizes the residual error between observed and predicted values¹⁹⁵. Due to its simplicity, interpretability, and low computational cost, LR was used as a baseline model against which more complex machine-learning approaches can be compared.

Decision tree (DT) is a simple supervised learning algorithm that predicts the target value by construction tree-like structure. At each node, the algorithm selects the split that best reduces prediction error, and the final prediction is obtained from the terminal leaf node reached by a given sample¹⁹⁶. DT models are easy to interpret and can capture nonlinear relationships and feature interactions, but they are often sensitive to data variation and may overfit if tree growth is not properly controlled¹⁹⁷.

RF is an ensemble learning algorithm that constructs multiple decision trees using different bootstrap samples and random subsets of input features for regression, classification, and related learning tasks¹⁹⁸. Each tree is built using randomly selected samples, and the final prediction is obtained by averaging (or weighted averaging) across all individual tree estimates, improving predictive accuracy and robustness.¹⁹⁹ RF performance can also be assessed using out-of-bag (OOB) samples, which correspond to the data points not included when building a given tree and therefore provide an internal estimate of the generalization error¹⁹⁹.

XGBoost is an efficient gradient-boosting decision-tree algorithm designed to achieve high predictive accuracy through regularization, optimized loss minimization, and parallelized computation²⁰⁰. XGBoost can be applied to regression and classification and has been widely adopted in engineering applications. Within the boosting framework²⁰¹, weak learners are added sequentially, with each new tree trained to reduce the residual errors of the current ensemble²⁰². As additional trees are incorporated, the loss function continues to decrease²⁰³, and the final prediction is obtained by summing the contributions from all trees in the model²⁰⁴.

LightGBM is a gradient-boosting framework that was developed to improve the computational efficiency and scalability of tree-based learning²⁰⁵. LightGBM accelerates training using histogram-based procedures that discretize continuous features into bins, thereby reducing memory usage and computation time.^{206,207} In addition, it adopts a leafwise split strategy rather than a levelwise strategy, allowing the construction of more complex trees and potentially improving predictive performance.²⁰⁸

Categorical Boosting (CatBoost) is a gradient-boosting algorithm designed to mitigate prediction bias and reduce target leakage, which is often associated with conventional

boosting^{209,210}. CatBoost can automatically process categorical-type information through permutation-based strategies, which helps to avoid manual encoding and improves robustness among diverse datasets and formats^{210,211}.

FT-Transformer is a transformer-based deep-learning architecture designed specifically for tabular data²¹². The model represents each feature as a token-like embedding and applies stacked self-attention layers to learn complex dependencies and interactions among input variables. Unlike conventional feedforward networks, FT-Transformer can capture both local and global relationships across features more effectively, which makes it suitable for structured datasets with nonlinear and interdependent patterns. Its architecture combines the flexibility of attention mechanisms with the ability to model high-dimensional tabular inputs in a data-driven manner.

TabM is a deep tabular learning model developed to improve predictive performance on structured datasets through efficient nonlinear feature transformation and representation learning²¹³. It is designed to capture complex relationships among predictors. By learning hierarchical feature representations through stacked blocks, TabM can model interactions that are difficult to express using conventional linear or tree-based approaches, which makes it a useful complement to ensemble learning methods for tabular regression problems.

Symbolic regression (SR) was implemented using the PySR package²¹⁴, which searches for explicit, human-interpretable analytical expressions that relate input features to target variables. PySR employs a multipopulation evolutionary search with an evolve–simplify–optimize loop to explore candidate equations and refine unknown scalar constants²¹⁵. The method is supported by a high-performance Julia backend that enables efficient evaluation and optimization of expressions²¹⁴. SR was used to derive closed-form equations linking the engineered dimensionless features to CO₂ trapping indices, providing a transparent alternative to black-box models.

3.6 Workflow methodology

The proposed methodology integrates physics-based reservoir simulation with data-driven modeling to predict CO₂ trapping mechanisms under uncertain reservoir and operational conditions. The simulation cases were generated using CMG-GEM with workflow automation and uncertainty sampling performed through CMOST. Each simulation corresponds to unique combination of reservoir properties, operational parameters, and geostatistical heterogeneity.

After completing the simulations and feature engineering, the dataset was split at the simulation case level to avoid any leakage of time step information between training and testing. This resulted in 418 cases for training and 105 for testing, following an 80/20 split. The training set was used for model development and hyperparameter tuning, whereas the test set was reserved for final performance evaluation. To ensure the models were both accurate and robust, hyperparameter optimization was carried out using Optuna²¹⁶ with 5-fold cross-validation, helping to minimize the risk of overfitting.

The model performance was quantified using the R^2 , RMSE, and nRMSE as defined in **Equations (21) - (23)**, which provide measures of predictive accuracy and error magnitude. Based on these metrics, the best predictive model and corresponding symbolic equation were selected to estimate the contributions of supercritical CO₂, dissolved CO₂, residually trapped CO₂, and mineralized CO₂ (%). The complete simulation–ML workflow is summarized in **Figure 12**.

$$RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i)^2} \quad (21)$$

$$nRMSE = \frac{RMSE}{target_{max} - target_{min}} \quad (22)$$

$$R^2 = 1 - \frac{\sum_{i=1}^n (y_i - \hat{y}_i)^2}{\sum_{i=1}^n (y_i - \bar{y})^2} \quad (23)$$

Where: y_i – actual value

$\hat{y}_i$ – predicted value

$\bar{y}$ – average actual value

$target_{max}$ – maximum value of target

$target_{min}$ – minimum value of target

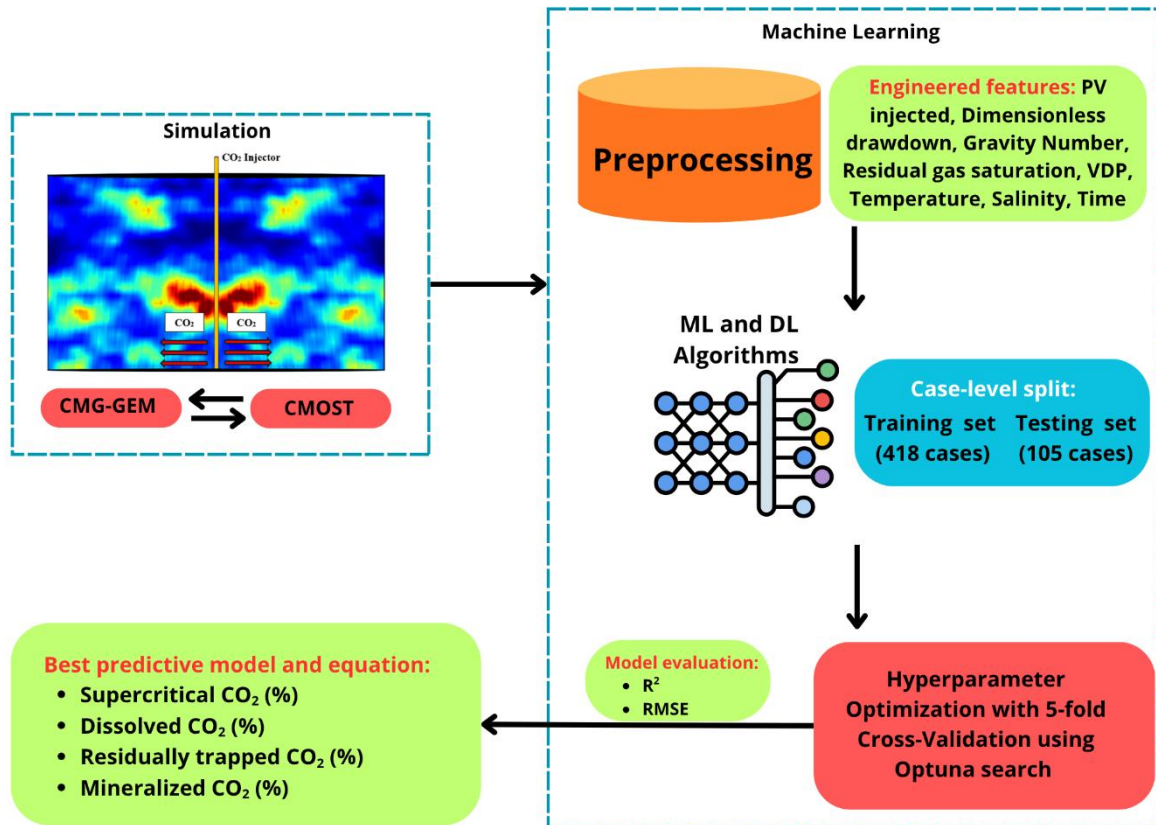


Figure 12. Flow chart of the methodology

4. RESULTS AND DISCUSSION

This chapter presents the main results of the developed physics-guided machine-learning framework for predicting CO₂ trapping behavior in heterogeneous deep saline aquifers. It first describes the hyperparameter tuning process and compares the predictive performance of the tested models. It then presents the symbolic-regression-derived equations and the feature-importance analysis used to interpret the governing controls of the four trapping indices. Finally, the chapter demonstrates the application of the best-performing TabM model through Monte Carlo analysis, sensitivity analysis, and inverse design for optimization of mineral trapping.

4.1 Hyperparameter tuning

Eight AI algorithms were optimized for predicting the four CO₂ trapping indices: supercritical, dissolved, residually trapped, and mineralized CO₂. Linear Regression (LR) was used as a baseline model and therefore was not subjected to hyperparameter tuning. Decision Tree (DT), Random Forest (RF), XGBoost (XGB), CatBoost, LightGBM, FT-Transformer, and TabM were tuned separately for each target. The hyperparameter optimization was performed using Optuna-based Bayesian optimization, which adaptively explores the search space by learning from the results of previous iterations and focuses on the regions that are more likely to contain the optimal hyperparameter combination. This makes the process more efficient than exhaustive grid search or random search, as it can identify comparably accurate hyperparameter combinations with fewer evaluations and lower computational cost.

For DT, the tuning focused on the main tree-structure parameters, including maximum depth, minimum samples required for splitting, minimum samples per leaf, and maximum features. RF was optimized through the number of estimators, maximum depth, minimum split and leaf constraints, feature subsampling, and bootstrap selection. For XGBoost, the search space included the number of estimators, maximum depth, learning rate, subsample ratio, column sampling ratio, minimum child weight, and the regularization parameters alpha, lambda, and gamma. LightGBM was tuned using its principal boosting and tree-complexity controls, including number of estimators, maximum depth, learning rate, number of leaves, minimum child samples, subsampling, column sampling, and regularization terms. CatBoost optimization included the number of iterations, tree depth, learning rate, L2 leaf regularization, random strength, and bagging temperature. For the deep tabular models, FT-Transformer was optimized using learning rate, weight decay, batch size, maximum epochs, and patience, while

TabM was tuned using similar training-related parameters together with the number of blocks. The optimized values reported in **Table 7** therefore correspond to the best-performing hyperparameter combination identified by Optuna for each model and each CO₂ trapping target.

In addition to these tuned models, symbolic regression (SR) was also employed in this study to derive explicit mathematical equations for the CO₂ trapping indices. However, unlike the other machine-learning models, SR was not included in the Optuna-based hyperparameter optimization framework because its main purpose was equation discovery rather than conventional predictive model tuning.

Table 7. Hyperparameter ranges and optimized values for each model

Model	Hyperparameter	Range	Supercritical CO ₂ (%)	Dissolved CO ₂ (%)	Residually trapped CO ₂ (%)	Mineralized CO ₂ (%)
LR	-	-	-	-	-	-
DT	max_depth	2-30	18	29	16	24
	min_samples_split	2-20	2	19	14	8
	min_samples_leaf	1-10	5	4	2	9
	max_features	[None, sqrt, log2]	None	None	None	None
RF	n_estimators	100-800	761	669	649	752
	max_depth	3-30	20	21	16	22
	min_samples_split	2-20	2	5	4	3
	min_samples_leaf	1-10	1	3	6	1
	max_features	[sqrt, log2, None]	log2	log2	log2	log2
	bootstrap	[True, False]	True	True	True	True
XGB	n_estimators	100-1200	1159	670	881	896
	max_depth	3-12	3	3	3	5

	learning_rate	1E-3-0.3]	0.0768445	0.13231	0.0363973	0.012746
	subsample	0.5-1.0	0.614262	0.859296	0.501107	0.858659
	colsample_bytree	0.5-1.0	0.693836	0.944456	0.794699	0.909396
	min_child_weight	1.0-20.0	18.7136	17.2662	15.7284	17.4989
	reg_alpha	1E-8-10.0	0.0011967 9	3.48258e-07	5.46987e-05	8.94394e-08
	reg_lambda	1E-8-10.0	1.6156	1.52612	6.08597e-06	0.0298723
	gamma	0.0-10.0	2.2784	3.77566	6.7652	1.99607
CatBoost	iterations	200-1500	1309	1077	1281	297
	depth	4-10	4	4	5	7
	learning_rate	1E-3-0.3	0.0554814	0.116329	0.0345749	0.0814322
	l2_leaf_reg	1.0-20.0	12.0374	3.35974	1.30784	5.19776
	random_strength	1E-8-10.0	6.53493	7.57281	7.40916	1.78546
	bagging_temperature	0.0-10.0	0.465091	3.34662	3.8185	8.7753
LightGBM	n_estimators	100-1200	888	1043	893	1052
	max_depth	3-16	3	3	7	11
	learning_rate	1e-3-0.3	0.107492	0.0817723	0.091892	0.00998333
	num_leaves	8-256	211	57	9	18
	min_child_samples	5-60	35	13	33	54
	subsample	0.5-1.0	0.588952	0.549816	0.541624	0.547995
	colsample_bytree	0.5-1.0	0.759396	0.641622	0.599476	0.733913
	reg_alpha	1E-8-10.0	0.076229	4.29801e-05	2.80104	2.79484e-07
	reg_lambda	1E-8-10.0	9.77673	0.00786714	2.676e-05	0.00032874
FT-Transformer	lr	1E-4 - 3E-3	0.0021443 1	0.00244157	0.00260757	0.001788
	weight_decay	1E-8 - 1E-3	0.0004634 6	4.54834e-06	7.73728e-06	3.0843e-06
	batch_size	[512, 1024, 2048, 4096]	512	512	512	1024
	max_epochs	[100, 150, 200]	200	150	200	200

	patience	[15, 25, 35]	15	35	15	35
TabM	lr	5E-4 - 3E-3	0.0019464 1	0.00263927	0.00220068	0.00287843
	weight_decay	1E-8 -1E-2	0.0043431 1	0.000593639	0.000249303	1.21004e-08
	batch_size	[512, 1024, 2048, 4096]	512	512	512	512
	max_epochs	[100, 150, 200]	150	200	100	100
	patience	[15, 25, 35]	25	25	15	15
	n_blocks	2-4	2	2	2	3
	Populations	12	12	12	12	12
SR	Population size	65	65	65	65	65
	Number of iterations	500	500	500	500	500

4.2 Model performance evaluation

Model performance metrics are shown in **Figure 13**, **Figure 14**, and **Figure 15**. **Figure 13(a)**, **Figure 14(a)**, and **Figure 15(a)** show the training performance, where most models demonstrate very high accuracy, characterized by R^2 values close to one and low root RMSE and nRMSE. Although training results are strong, the testing performance shown in **Figure 13(b)**, **Figure 14(b)**, and **Figure 15(b)** provides a more reliable measure of model generalization.

On the testing dataset, the TabM model consistently outperforms the other approaches across all trapping mechanisms. As shown in **Figure 13(b)**, TabM demonstrates the highest R^2 values: 0.957 for supercritical CO_2 , 0.964 for dissolved CO_2 , 0.942 for residually trapped CO_2 , and 0.930 for mineralized CO_2 . The RMSE results in **Figure 14(b)** further support this result, where TabM shows the lowest prediction errors for all targets, with RMSE values of approximately 3.179, 2.029, 3.252, and 0.537, respectively, which indicates stable and accurate predictions over the entire data range.

The NRMSE results in **Figure 15(b)** also confirm this trend. TabM gives the lowest normalized prediction errors, with values of approximately 4.285, 4.229, 4.901, and 3.273, respectively. CatBoost, FTTransformer, LightGBM, and XGBoost also demonstrate strong

predictive capability on the test data; however, their errors are consistently higher than those of TabM, particularly for residually trapped CO₂.

Cross-validation results shown in **Figure 13(c)**, **Figure 14(c)**, and **Figure 15(c)** further confirm the same overall pattern, where TabM retains the highest cross-validated R² and the lowest cross-validated RMSE and nRMSE for all four trapping indices.

Overall, the predictive accuracy benchmark can be summarized as TabM > CatBoost ≈ FTTransformer > LightGBM ≈ XGBoost > RF > SR > DT > LR, TabM provides the most accurate and reliable predictions on unseen data, making it the most suitable model for estimating CO₂ trapping indices.

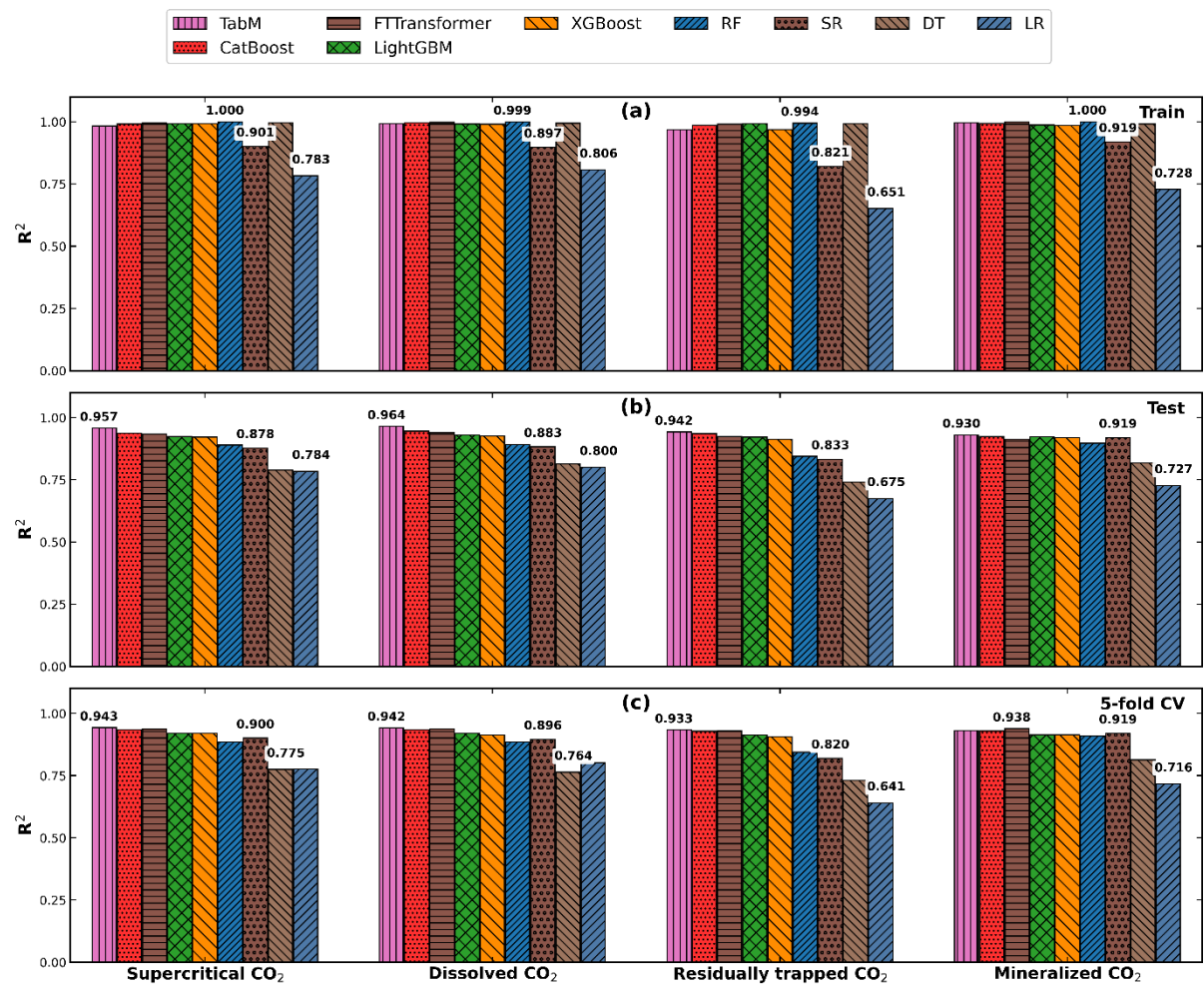


Figure 13. Comparison of model performance in terms of R²: (a) training dataset, (b) testing dataset, and (c) cross-validation score

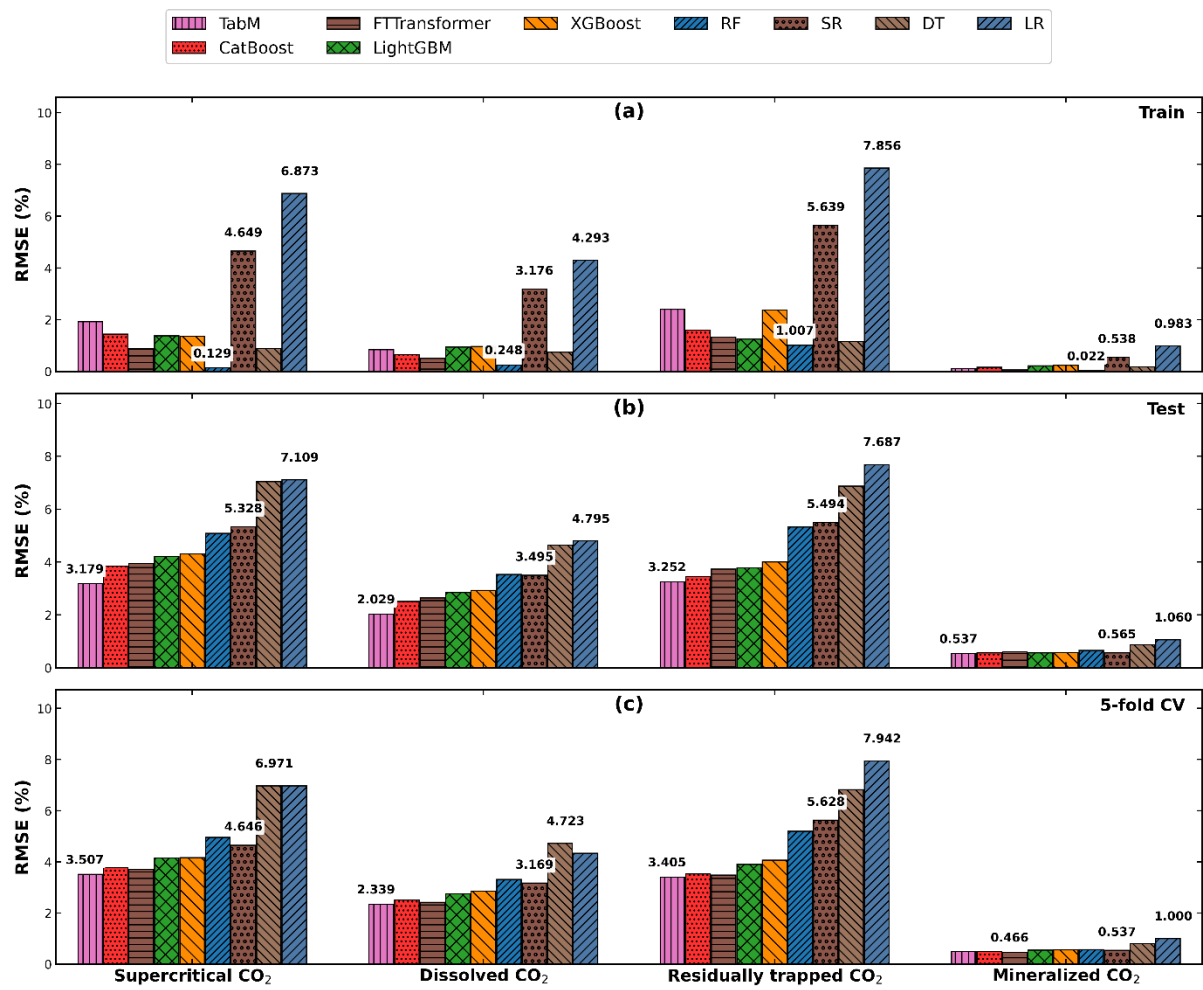


Figure 14. Comparison of model performance in terms of RMSE: (a) for the training dataset, (b) for the testing dataset, and (c) CV score

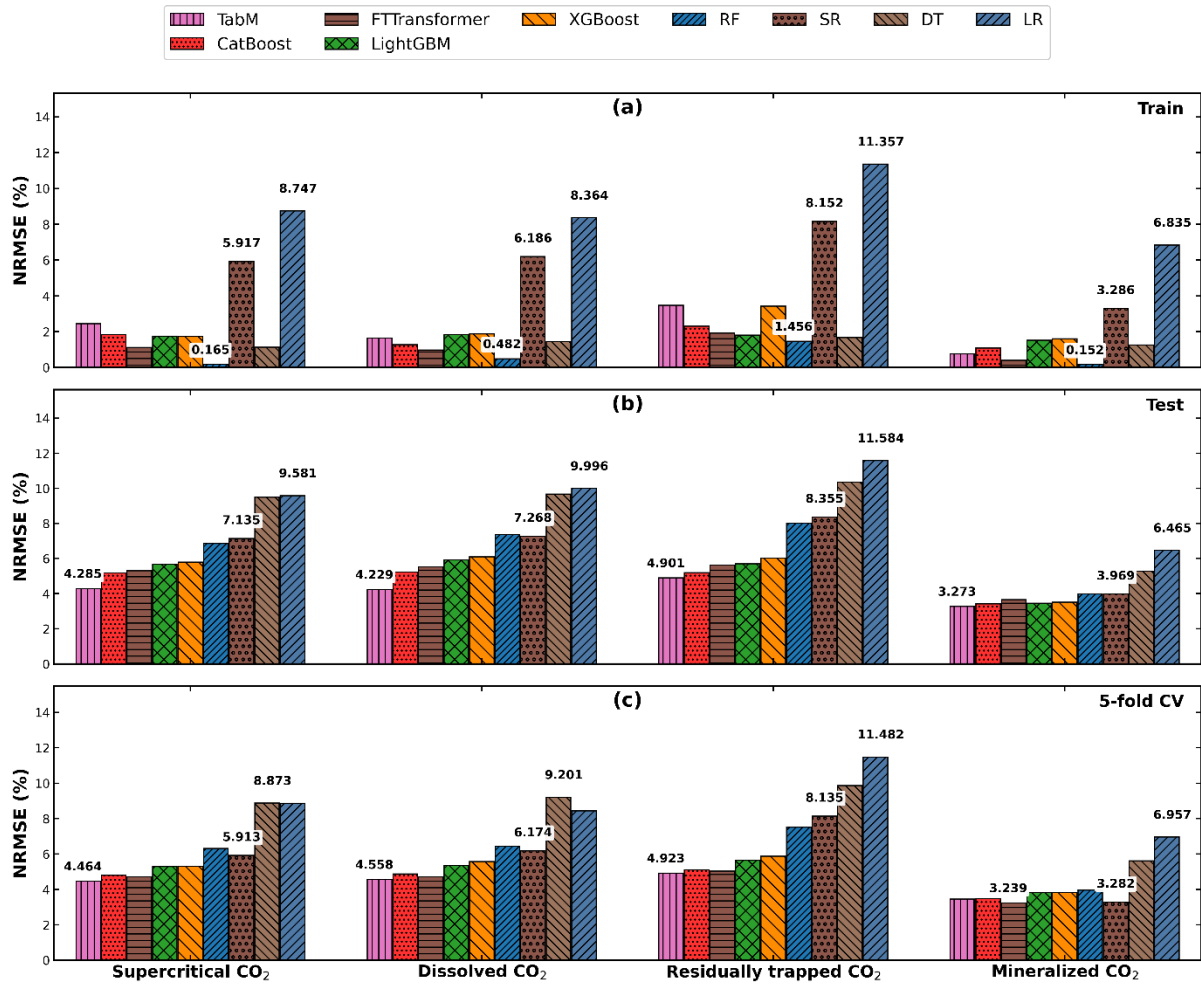
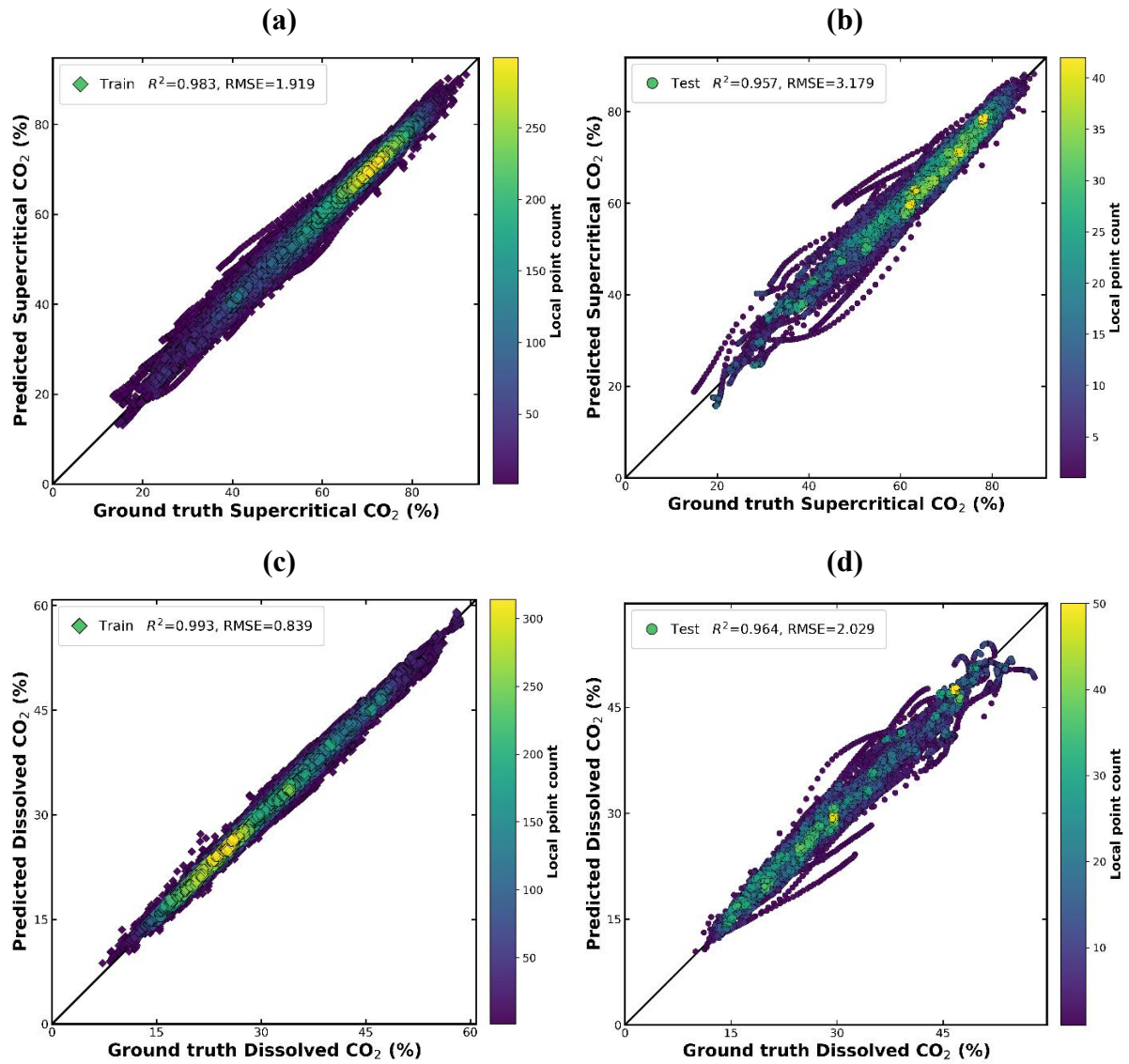


Figure 15. nRMSE values for each model and each target: (a) for the training dataset, (b) for the testing dataset, and (c) CV score

The actual-versus-predicted plots of the TabM model are shown in **Figure 16**. For supercritical CO₂, the predictions are tightly distributed around the ideal $Y = X$ line, with high accuracy achieved in both splits (train: $R^2 = 0.983$, RMSE = 1.919; test: $R^2 = 0.957$, RMSE = 3.179). A similarly close agreement is observed for dissolved CO₂, where the model delivers the highest testing accuracy among the four targets (train: $R^2 = 0.993$, RMSE = 0.839; test: $R^2 = 0.964$, RMSE = 2.029), with only limited scatter across the prediction range. For residually trapped CO₂, the predictions remain well aligned with the reference line, although the spread is slightly wider than for supercritical and dissolved fractions (train: $R^2 = 0.968$, RMSE = 2.393; test: $R^2 = 0.942$, RMSE = 3.252). This suggests that residual trapping is harder to predict, most likely because it is more sensitive to heterogeneity-driven flow variations and local plume redistribution. For mineralized CO₂, the TabM model also shows very strong predictive performance, particularly on the training set (train: $R^2 = 0.997$, RMSE = 0.107), while the testing results remain robust (test: $R^2 = 0.930$, RMSE = 0.537). The somewhat larger relative

scatter in the testing plot at higher values is reasonable given the narrower target range and the strong concentration of data at low mineralization values. Overall, these plots demonstrate that TabM provides accurate and reliable predictions across all trapping mechanisms, with the strongest generalization observed for dissolved and supercritical CO₂, while residual and mineralized fractions remain slightly more challenging due to their greater sensitivity to reservoir heterogeneity and distribution of target values.



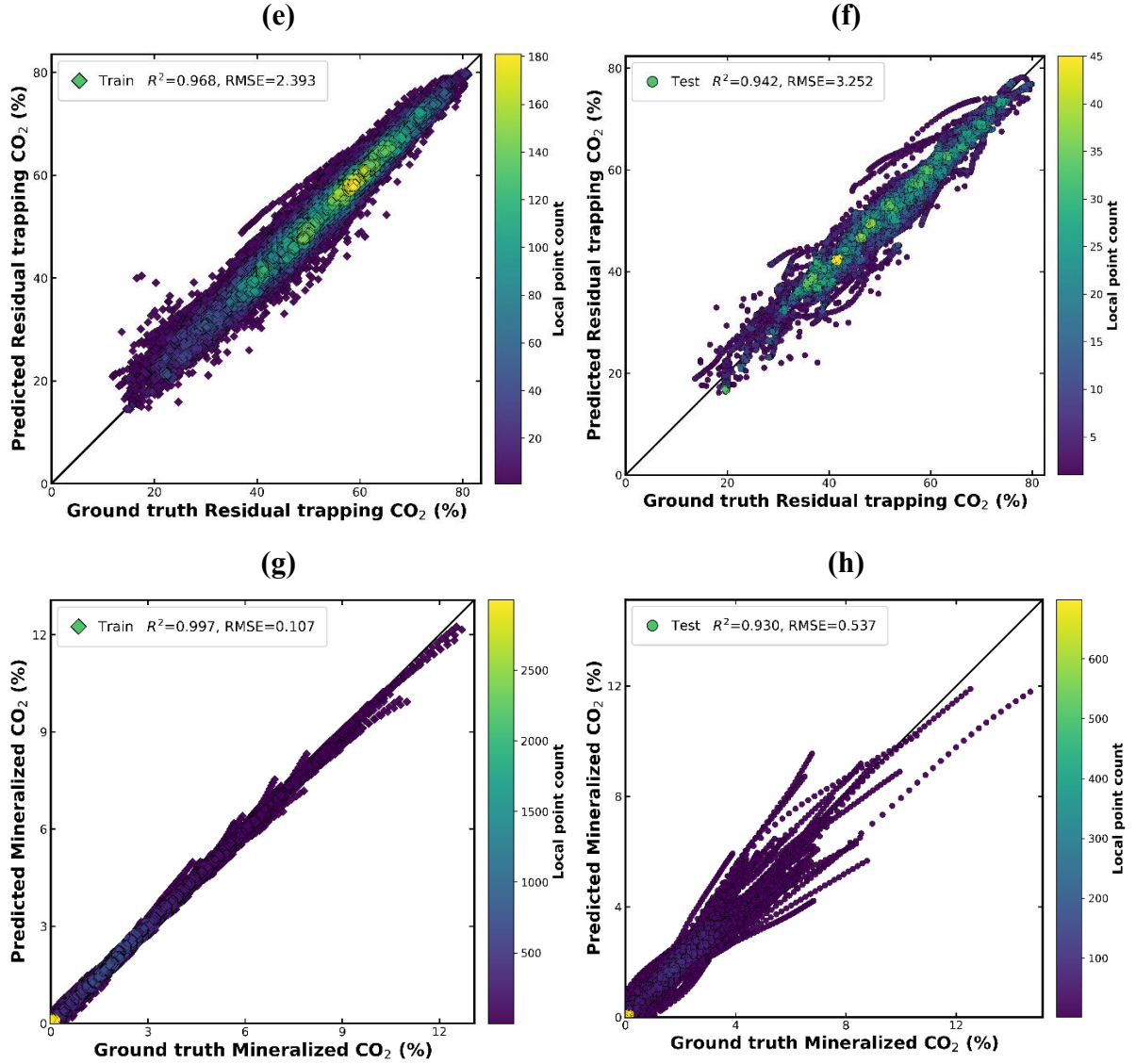


Figure 16. Actual vs predicted plots for TabM model and each target: (a) train and (b) test of Supercritical CO₂ (%), (c) train and (d) test of Dissolved CO₂ (%), (e) train and (f) test of Residually trapped CO₂ (%), (g) train and (h) test of Mineralized CO₂ (%).

Additionally, **Figure 17** presents a comparison between the CO₂ trapping indices predicted by the TabM model and the actual values obtained from the numerical simulation for a newly generated case that was not used in either the training or testing process. TabM model captures the overall trend and magnitudes of the supercritical, dissolved, residually trapped, and mineralized CO₂ fractions with good agreement with the simulation results. The TabM model demonstrates strong agreement with simulation data across all trapping mechanisms over the 200-years period. These results indicate that the proposed ML model can reliably estimate the time-dependent evolution of CO₂ different trapping states.

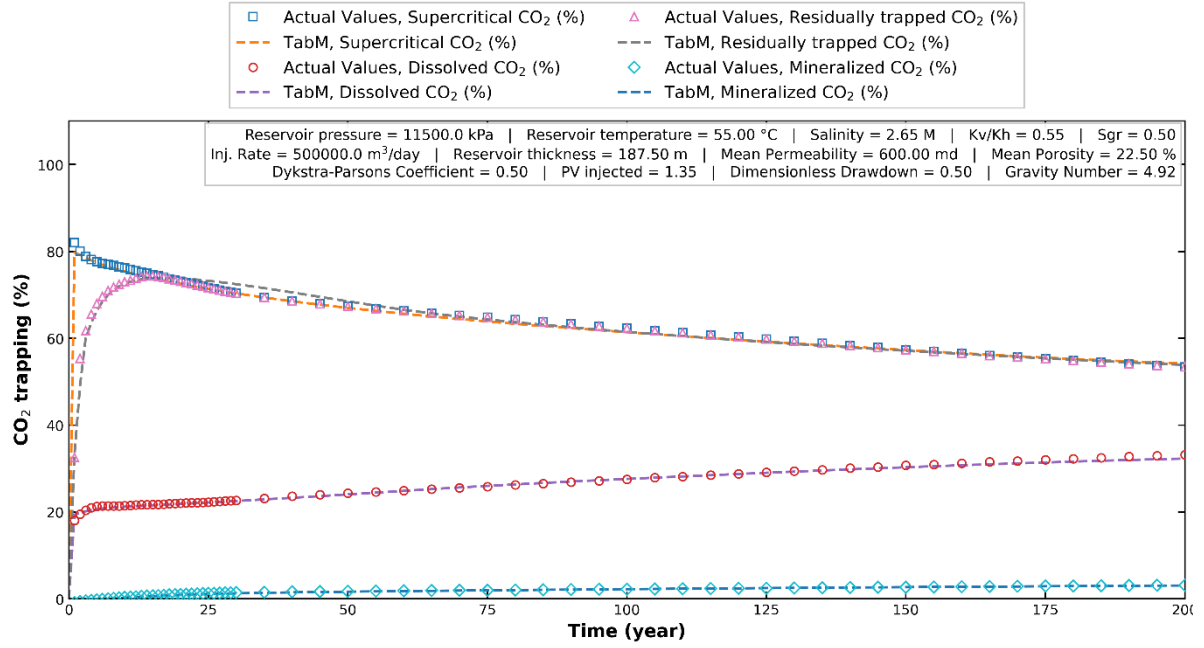


Figure 17. Comparison of the CMG-simulated and TabM predicted supercritical CO₂ index, dissolved CO₂ index, residual trapping index, and mineral trapping index.

4.3 Symbolic regression-derived equations

As mentioned earlier, an SR approach based on genetic expression programming (GEP) was employed in this study to derive explicit analytical expressions for predicting the CO₂ trapping indices. Unlike fixed-form polynomial models, SR does not assume a predefined equation structure. Instead, as an evolutionary algorithm, GEP searches for suitable mathematical relationships by generating, modifying, and evaluating a large population of candidate expressions over successive generations. The resulting equations are not constrained to include all input variables; rather, only those variables that contribute meaningfully to predictive accuracy are preserved, which leads to compact and interpretable equation.

Using this procedure, closed-form equations were obtained for the four trapping components - supercritical, dissolved, residually trapped, and mineralized CO₂ fractions - presented in **Equations (24) – (26)**, respectively.

$$SCI = Q_d \times (2D_d - 0.498G - 5.275) + \frac{V_{DP}}{G^2} - (19.308 - 6.994H_g - 1.084S) \times \log\left(t + \frac{37.202}{Q_d}\right) + 133.816 \quad (24)$$

$$\begin{aligned}
\mathbf{STI} = & -21.524H_g - 4.735S + (Q_d + 2.377) \times (\log(S + t) - 3.159) \\
& + 2.589 \log(G) + 42.403 + \frac{1}{Q_d^2}
\end{aligned} \tag{25}$$

$$\begin{aligned}
\mathbf{RTI} = & -1.576\sqrt{G} \times (Q_d + 0.188) + 4.142S - 0.111t \times (D_d + H_g) + (D_d + H_g)^3 \\
& + 35.467 \times (0.489H_g + 1)^3 - \frac{37.497}{t}
\end{aligned} \tag{26}$$

$$\begin{aligned}
\mathbf{MTI} = & (0.035 - 0.026H_g) \times \left(0.060 - \frac{0.024}{G + 0.540}\right) \\
& \times (1.833Q_d \times (G + 11.319) + T_r) \times \log(t)^2 - \frac{2.368}{Q_d^2 + t}
\end{aligned} \tag{27}$$

1046 where SCI, STI, RTI, and MTI denote the supercritical, dissolved, residually trapped, and
 1047 mineralized CO₂ fractions (in %), respectively; D_d is the dimensionless drawdown parameter,
 1048 Q_d is the injected pore volume; G is the gravity number; H_g is the residual gas saturation; S is
 1049 brine salinity; t is elapsed time; T_r is the reservoir temperature; and VDP is the Dykstra-
 1050 Parsons coefficient.

1051 **Figure 17** compares the CO₂ trapping indices predicted by the derived SR equations
 1052 with the actual values obtained from the numerical simulation for a newly generated case that
 1053 was not used during models training. The SR equations successfully reproduce the overall
 1054 trends and magnitudes of the supercritical, dissolved, residually trapped, and mineralized CO₂
 1055 fractions in good agreement with the simulation results. Strong agreement is observed across
 1056 all trapping mechanisms throughout the 200-year period, indicating that the derived equations
 1057 are capable of reliably describing the time-dependent evolution of the various CO₂ trapping
 1058 states.

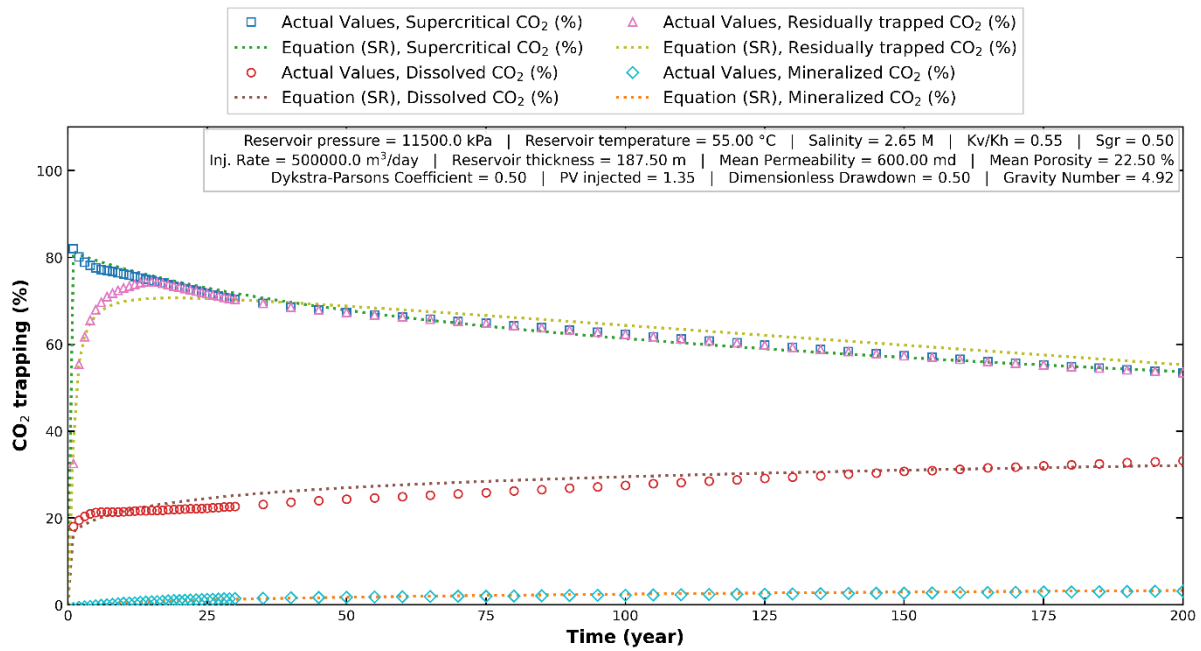


Figure 18. Comparison of the CMG-simulated and estimated by equation supercritical CO₂ index, dissolved CO₂ index, residual trapping index, and mineral trapping index.

It is important to note that residual trapping can become progressively more important over time and may, in some settings, exceed both structural and solubility trapping. Once CO₂ injection is terminated, the continuous supply of CO₂ to the storage formation stops, which weakens the displacement of brine by supercritical CO₂ and reduces competition for pore space between the CO₂ and the aqueous phase²¹⁷. As fluid motion diminishes, supercritical CO₂ is more readily trapped as disconnected ganglia within the pore network, which contributes to the residual trapping³⁸. The system also tends toward quasi-equilibrium conditions in the post-injection period, under which capillary forces and interfacial tension between supercritical CO₂, brine, and the rock matrix become more dominant²¹⁸. These forces suppress further CO₂ migration and favor entrapment in pores that are smaller and less connected. Consequently, the redistribution of CO₂ into pore spaces where capillary effects are stronger can further enhance residual trapping over time²¹⁹.

4.4 Analysis of feature importance

Additionally, the relative influence of the governing input parameters on each CO₂ trapping mechanism was assessed using SHAP. **Figure 19** presents the SHAP beeswarm plots for the TabM models predicting the supercritical, dissolved, residually trapped, and mineralized CO₂ fractions. Points located to the right (left) of the vertical zero line indicate a

positive (negative) contribution of a given feature to the predicted trapping index. The color scale represents the magnitude of the feature value. The horizontal spread of SHAP values reflects the impact of each feature on the model output, while the vertical order is indicated by the relative feature importance.

For the supercritical CO₂ fraction, storage time is the most influential parameter, followed by salinity. Higher salinity suppresses CO₂ dissolution in brine, which leads to increased fraction of CO₂ remaining in the supercritical state and contributing to structural trapping of CO₂²²⁰. Gravity number and injected pore volume also exhibit a noticeable influence, which indicates that the balance between buoyancy-driven vertical segregation and cumulative injection intensity governs both the persistence and redistribution rate of supercritical CO₂. This behavior is consistent with prior findings showing that buoyancy-dominated systems promote faster plume migration but limit the extent of immobilization¹²⁹.

Solubility trapping is primarily controlled by brine salinity, consistent with the salting-out effect reported in previous experimental and numerical studies^{221,222}. Secondary influences include storage time and injected pore volume, reflecting the importance of prolonged CO₂–brine contact and exposure duration for dissolution processes. The comparatively weak contribution of permeability heterogeneity (V_{DP}) suggests that fluid properties and operational timescales dominate solubility trapping rather than spatial variability.

Residual trapping is strongly affected by residual gas saturation and time, highlighting the role of hysteresis-related immobilization following injection. This dependence on saturation history and timing is consistent with classical observations that lower gravity-number conditions favor greater residual trapping, whereas higher gravity-number systems reach immobilization more rapidly but at lower ultimate trapped fractions¹²⁹.

Mineral trapping is primarily governed by storage time and injected pore volume, reflecting its inherently slow and cumulative nature. Additional contributions from gravity effects and temperature are observed, with increased temperature promoting mineralization through enhanced reaction kinetics^{223,224}. In contrast, higher residual gas saturation and stronger pressure drawdown tend to suppress mineral trapping by limiting sustained CO₂–brine contact⁴².

The limited influence of permeability heterogeneity, represented by the Dykstra–Parsons coefficient, is consistent with previous studies⁴⁶. In the present work, this behavior can be attributed to the adopted modeling strategy, in which both the magnitude of

heterogeneity (V_{DP}) and the spatial distribution of permeability vary from case to case. As a result, heterogeneity is represented as a truly stochastic process, introducing randomness that makes the impact of permeability variability on individual trapping mechanisms less deterministic and more difficult for the machine-learning model to isolate. This representation is considered more realistic than analyses based on a single, fixed permeability architecture in which heterogeneity is varied only by increasing or decreasing permeability contrast while preserving the same spatial geometry. The influence of VDP would likely appear more pronounced in such idealized cases; however, these scenarios are less representative of natural subsurface systems.

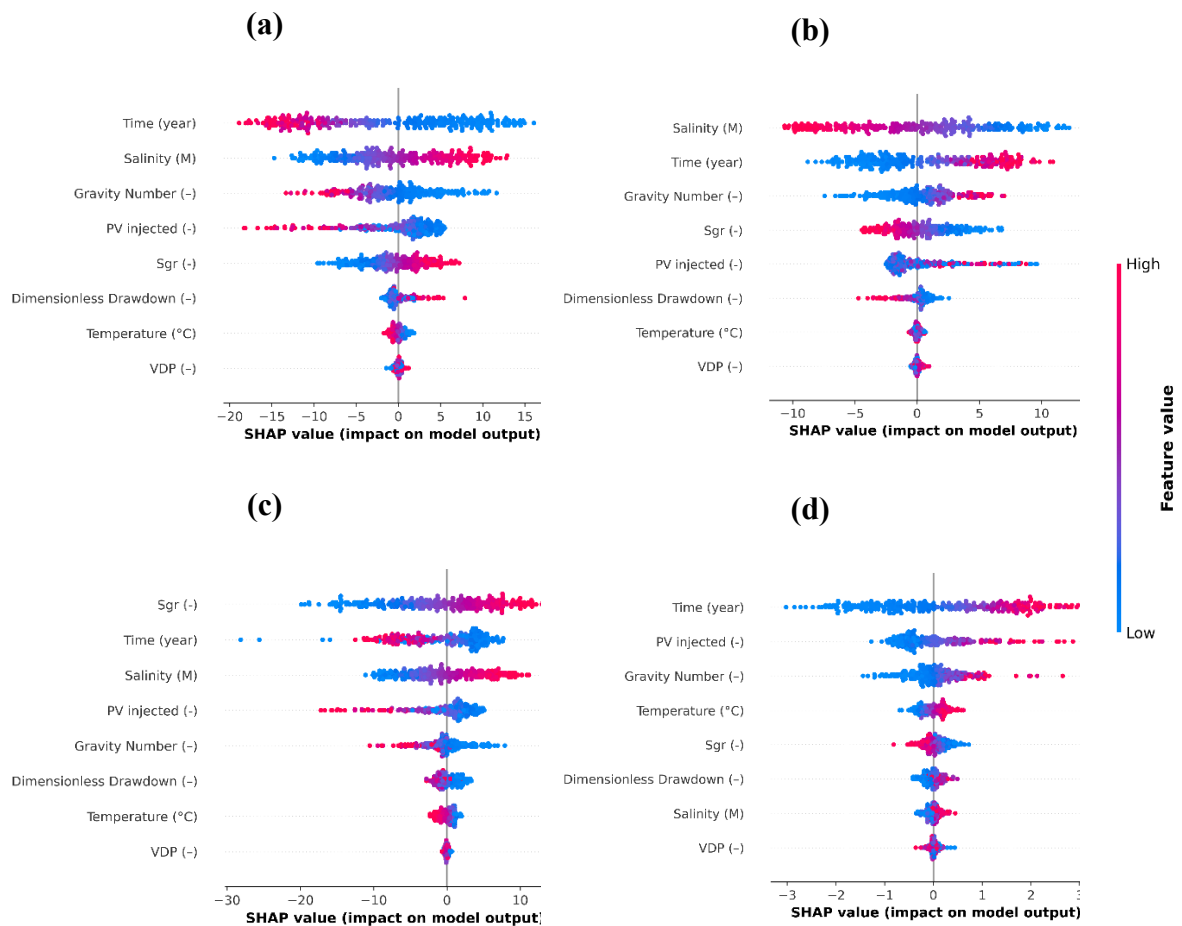


Figure 19. SHAP plots for (a) supercritical, (b) solubility, (c) residual, and (d) mineral-trapping fractions of CO₂.

4.5 Application of TabM model

4.5.1 Monte Carlo Analysis

Figure 20 shows the Monte Carlo uncertainty curves for the four CO₂ trapping mechanisms over the 200-year period. In this analysis, 5,000 Monte Carlo realizations were generated to quantify the effect of input uncertainty on the predicted trapping behavior.

The supercritical CO₂ fraction decreases with time, which indicates progressive reduction of the mobile phase. The dissolved and mineralized fractions increase continuously as dissolution and long-term stabilization become more important. Residual trapping increases rapidly during the early stage, reaches a maximum, and then gradually declines. This reflects the redistribution of CO₂ among the trapping mechanisms over time.

The shaded P10-P90 and P25-P75 intervals further demonstrate that uncertainty remains significant throughout the simulation period, particularly for the supercritical and residually trapped fractions.

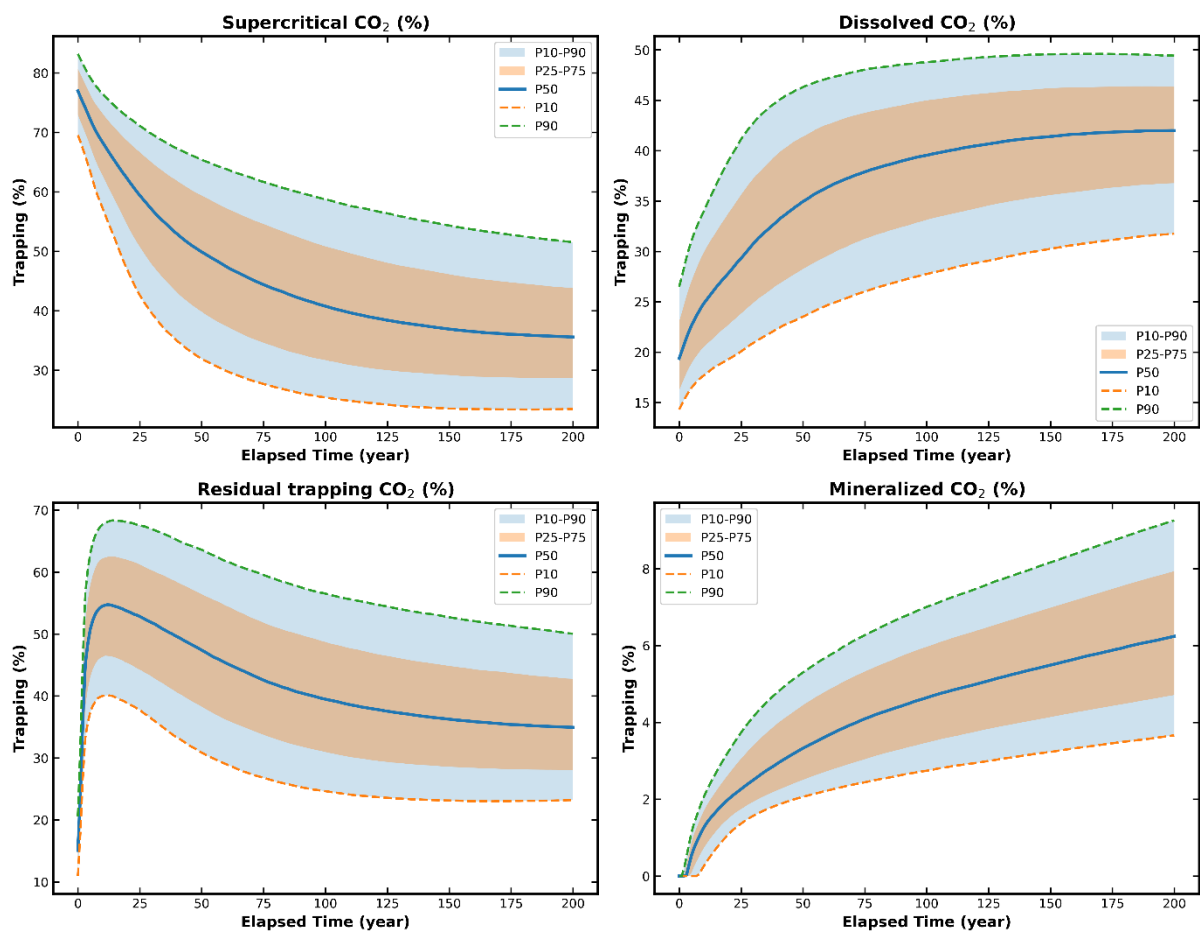


Figure 20. Temporal Monte Carlo analysis for supercritical, dissolved, residual, and mineralized CO₂ fractions

The final probabilistic outcomes at 200 years are summarized in **Figure 21**. For supercritical CO₂, the P90, P50, and P10 values are 23.48%, 35.59%, and 51.52%, respectively. For dissolved CO₂, the corresponding values are 31.77%, 41.99%, and 49.43%. For residual trapping, the P90, P50, and P10 values are 23.21%, 34.93%, and 50.04%, respectively, and mineralized CO₂ values of 3.66%, 6.24%, and 9.26%. These distributions confirm that dissolved and residual trapping represent major contributions to long-term storage, whereas mineral trapping develops more gradually and within a narrower range. The ML-based Monte Carlo uncertainty propagation required only 42.598 s. In contrast, conducting a comparable uncertainty study using repeated full-physics reservoir simulations would likely require weeks of computational time.

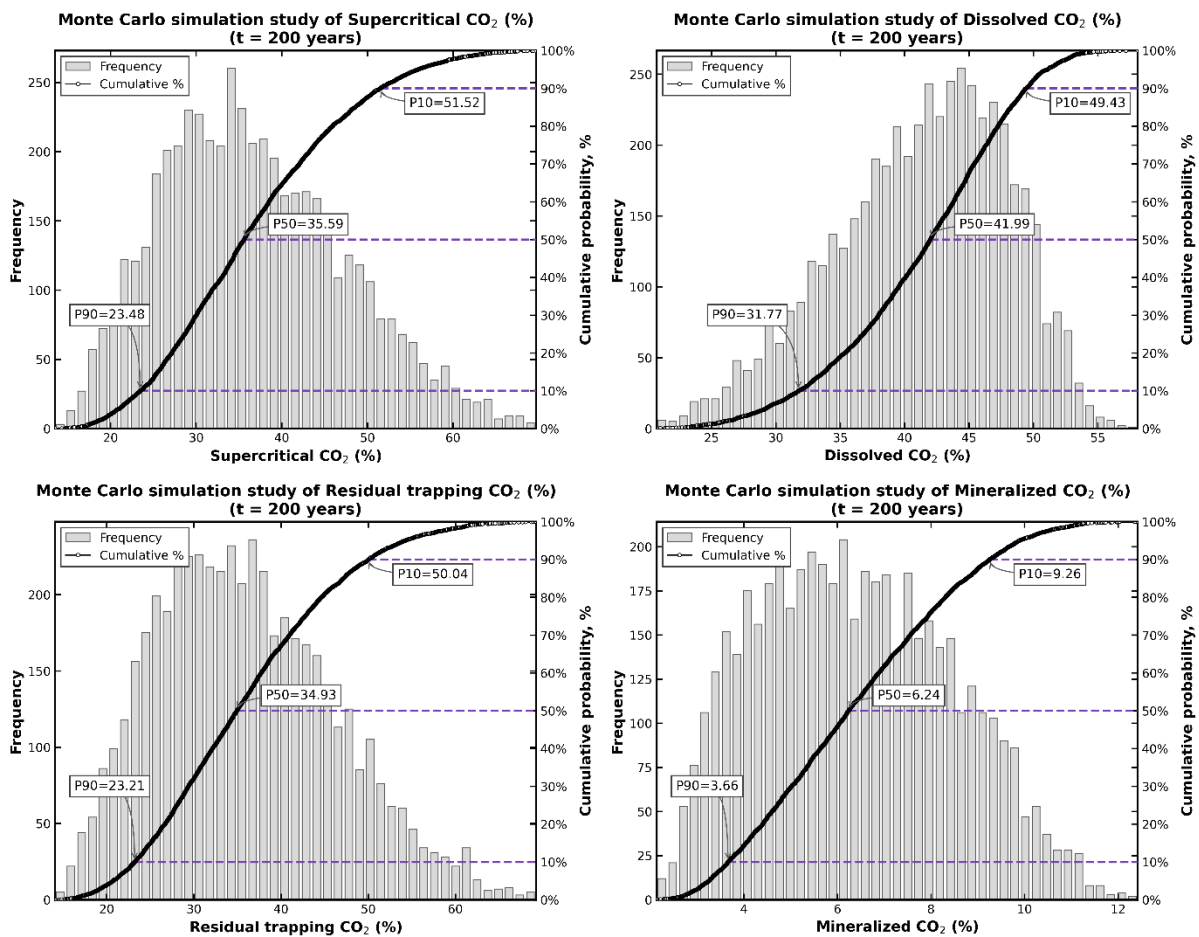


Figure 21. Frequency and cumulative probability distributions of the four CO₂ trapping components at 200 years obtained from Monte Carlo simulation

4.5.2 Sensitivity analysis

A sensitivity analysis was conducted using the TabM model to evaluate the influence of the most impactful input variables on the predicted CO₂ trapping behavior, and the obtained

trends were further validated against the numerical simulation model. The validation data were not previously used in the training or testing datasets. The analysis focused on salinity, gas hysteresis coefficient, reservoir temperature, as these variables showed the strongest effect on the trapping indices, both by feature importance analysis and in experimental studies^{40,42}. The TabM predictions were compared with the corresponding simulation results. The close agreement between the machine-learning predictions and the numerical simulation outcomes confirms that the TabM model was able to capture the main sensitivity trends of the system with reasonable reliability.

4.5.2.1 Effect of salinity

As shown in **Figure 22**, increased salinity led to a clear reduction in dissolved CO₂, with a larger fraction of CO₂ remained in the supercritical phase and was subsequently trapped through residual trapping mechanism. This trend is consistent with the salting-out effect, where dissolved salts reduce the solubility of CO₂ in brine. This limits the amount of free water available for dissolution. Similar observations have been reported in experimental and thermodynamic studies of CO₂ solubility in saline systems^{225,226}.

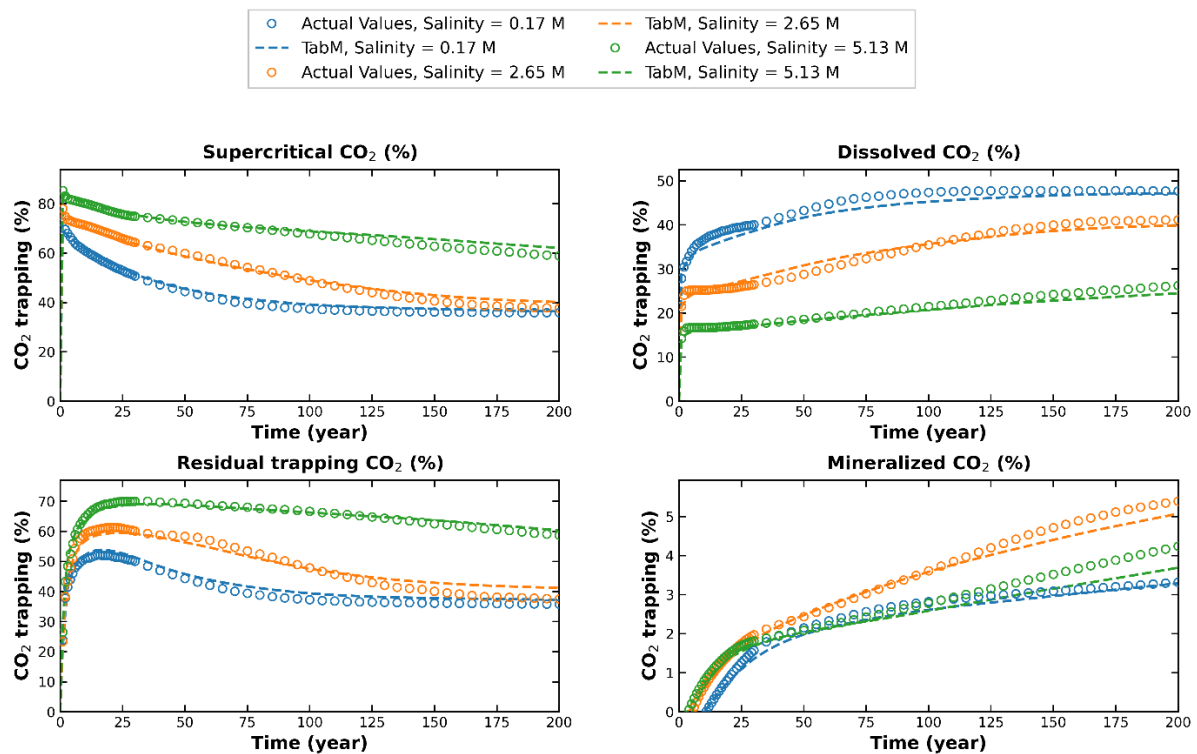


Figure 22. Sensitivity of CO₂ trapping indices to salinity as predicted by the TabM model and validated against the numerical simulation

4.5.2.2 Effect of Gas Hysteresis Coefficient (S_{gr})

Figure 23 shows that increasing the gas hysteresis coefficient, S_{gr} , led to a clear increase in residual trapping, while the dissolved and mineralized CO_2 fractions decreased. The supercritical CO_2 fraction also remained higher at larger S_{gr} values. This behavior is consistent with the physics of relative permeability hysteresis: during imbibition, brine re-enters the pore space, disconnects the nonwetting CO_2 phase, and leaves part of it immobilized as residual gas. In Land-type trapping formulations, stronger hysteresis or larger residual-gas parameters increase the amount of CO_2 that becomes immobile after plume retreat²²⁷. Experimental studies at reservoir conditions have confirmed that trapped CO_2 saturation increases with the maximum CO_2 saturation reached and that hysteresis strongly controls the CO_2 /brine relative-permeability response. In the present sensitivity analysis, the lower dissolved and mineralized fractions at higher S_{gr} likely reflect reduced mobile CO_2 -brine contact and less effective mass transfer once a larger portion of CO_2 becomes residually trapped.

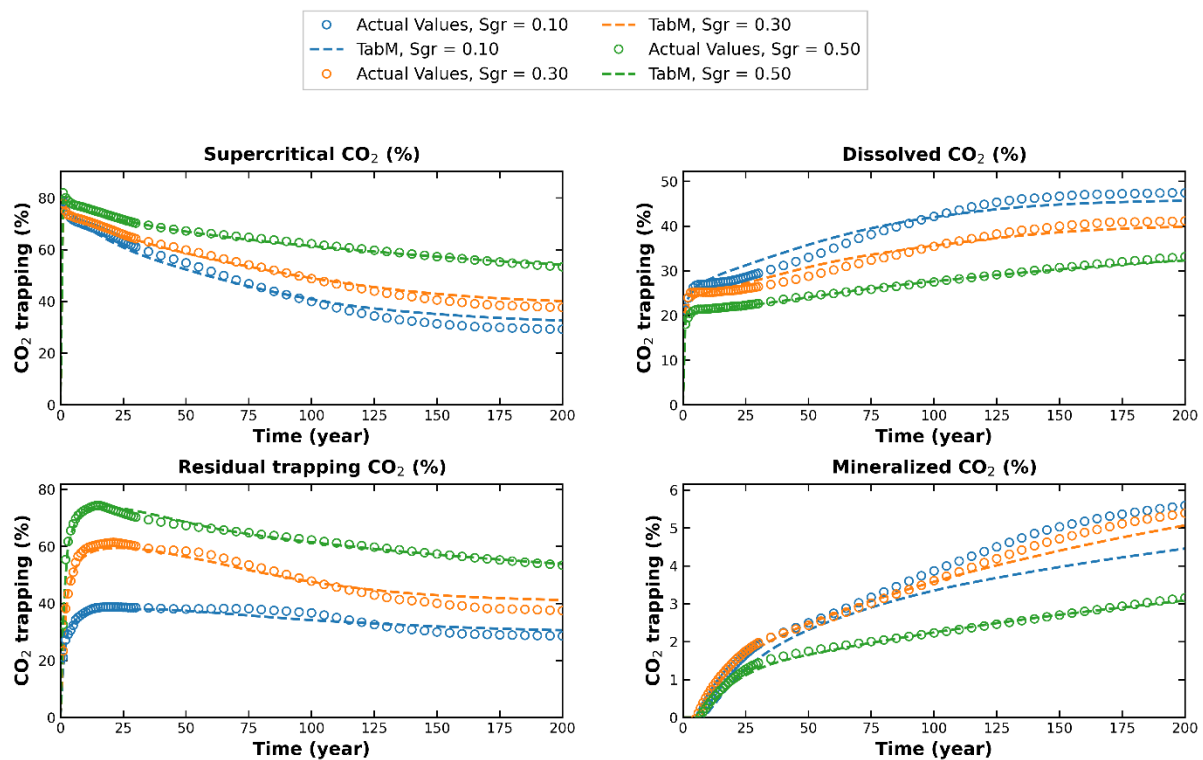


Figure 23. Sensitivity of CO_2 trapping indices to the gas hysteresis coefficient (S_{gr}) as predicted by the TabM model and validated against the numerical simulation

4.5.2.2 Effect of reservoir temperature

As shown in **Figure 24**, increasing reservoir temperature reduced the supercritical and residual-trapping CO_2 , while the dissolved and mineralized CO_2 increased over time. Although

experimental solubility measurements show that CO₂ solubility in NaCl brine generally decreases as temperature increases under fixed pressure and salinity conditions, reservoir-scale behavior can differ because temperature may intensify thermohaline fingering and convective-reactive transport, thereby enhancing effective CO₂ dissolution in dynamic systems^{224,231}. Since mineral trapping develops from dissolved CO₂ through subsequent CO₂-brine-rock reactions, the higher dissolved CO₂ fraction at elevated temperature can also explain the corresponding increase in mineralized CO₂ observed in this figure²³².

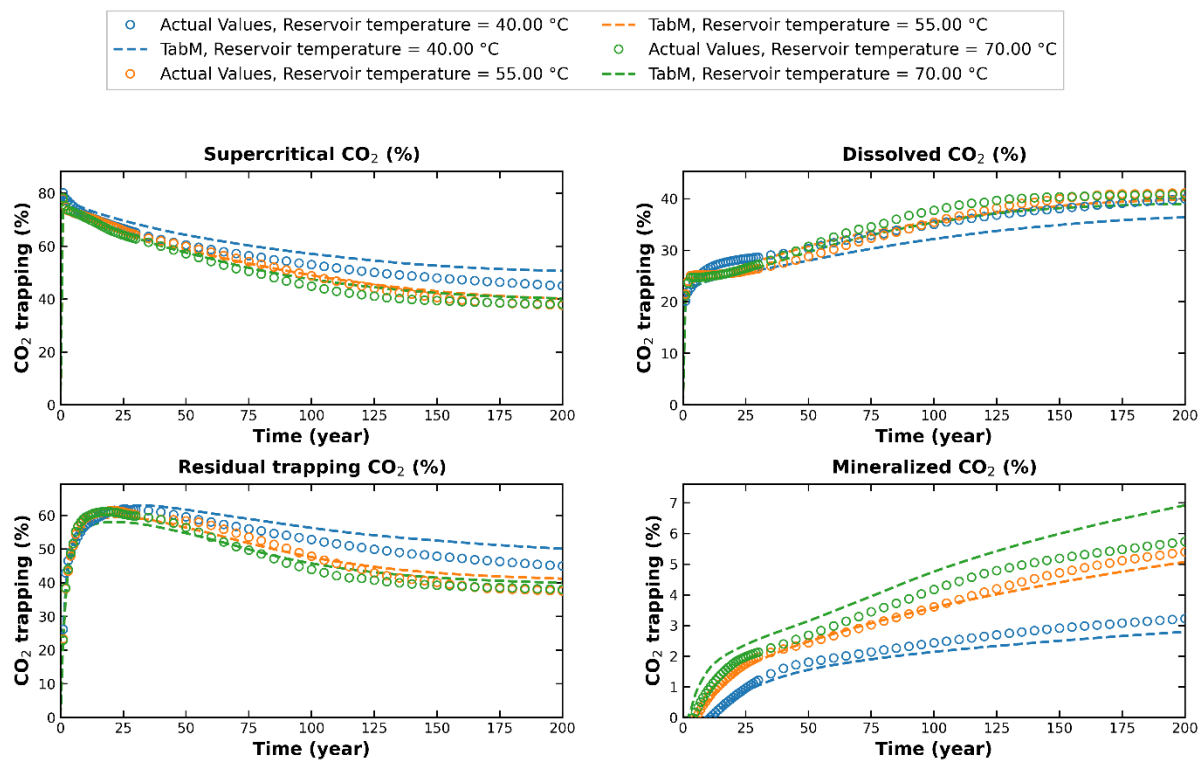


Figure 24. Sensitivity of CO₂ trapping indices to reservoir temperature as predicted by the TabM model and validated against the numerical simulation

4.5.3 Inverse design for optimization mineral trapping

Within CCS, the long-term reliability of the different CO₂ trapping mechanisms varies considerably, with mineral trapping recognized as the most stable and practically irreversible form because CO₂ is converted into solid carbonate minerals through geochemical reactions⁴⁸. Operating over centennial to millennial time scales, this mechanism significantly reduces the risk of CO₂ remigration or leakage. Therefore, a higher degree of mineralization corresponds to greater storage security, which supports evaluating system performance over a 200-year time scale in this study.

To identify the input conditions associated with enhanced mineral trapping, an inverse-design workflow was carried out using the best-performing machine-learning model selected during model evaluation, namely TabM. In this analysis, the optimization space was defined by seven input variables: injection rate, dimensionless drawdown, reservoir heterogeneity coefficient, residual gas saturation parameter, gravity number, reservoir temperature, and salinity. The simulation time was fixed at 200 years to ensure consistent comparison of long-term mineralization performance across all evaluated cases. Within the prescribed bounds of these variables, 200,000 Sobol-sampled scenarios were generated and evaluated by the trained model to predict the mineralized carbon dioxide fraction. The predicted outputs were then ranked, and the top 10% most mineralized cases were extracted to define the high-mineralization operating window. Accordingly, the threshold for this subset corresponds to 11.13% mineralization.

Table 8 shows the percentile distribution of the input variables for the most highly mineralized cases obtained from the inverse optimization analysis. The identified solutions are grouped within a narrow region. The results show that favorable cases are characterized by intermediate-to-high PV injected values, with a median of 5.52 and an interquartile range of 4.72–6.12, together with moderate dimensionless drawdown values centered around 0.86. In addition, the preferred range of VDP (0.26–0.65) suggests that moderate heterogeneity is advantageous, while Sgr values of 0.15–0.30 indicate that excessive gas immobilization is not required for strong mineral conversion. The optimal region is further associated with relatively high gravity number, temperature, and salinity, whose medians are 23.88, 61.06 °C, and 3.88 M, respectively. Therefore, this design provides a practical basis for the definition of screening criteria and recommended operating ranges for mineral-trapping-oriented CCS design.

Table 8. Percentile ranges of input parameters for cases with mineralization percentage above 11.13%

Variable	5%	25%	50%	75%	95%	Search space
PV injected (-)	3.42	4.72	5.52	6.12	6.52	0.36–6.62
Dimensionless Drawdown (-)	0.36	0.64	0.86	1.07	1.31	0.145–1.403
VDP (-)	0.14	0.26	0.44	0.65	0.84	0.108–0.892
Sgr (-)	0.11	0.15	0.21	0.30	0.42	0.104–0.496
Gravity Number (-)	10.25	18.14	23.88	28.80	33.38	0.405–34.86
Temperature (°C)	46.63	55.18	61.06	65.67	68.91	40.286–69.713
Salinity (M)	1.65	3.00	3.88	4.54	4.98	0.2204–5.083

To examine mineral trapping under highly conservative conditions, all non-selected input variables were fixed at their respective 5th percentile values, while the simulation time was fixed at 200 years. Based on the prior feature-importance analysis, the three most influential variables for this case, namely PV injected, Gravity Number, and temperature, were selected as the only free design variables. A three-dimensional inverse-design search was then performed. All remaining inputs were kept unchanged. The TabM model was used to predict the corresponding mineralized CO₂ fraction for each sampled combination, and the resulting response space was visualized in the PV injected-Gravity-temperature domain, as shown in **Figure 25**. The obtained distribution shows that mineralization increases toward the region of simultaneously higher PV injected, higher Gravity Number, and higher temperature, with the best scenarios reaching approximately 10% mineralized CO₂. This indicates that, even when the other parameters are held at conservative low-percentile conditions, coordinated adjustment of these three dominant controls can still noticeably improve mineral trapping performance.

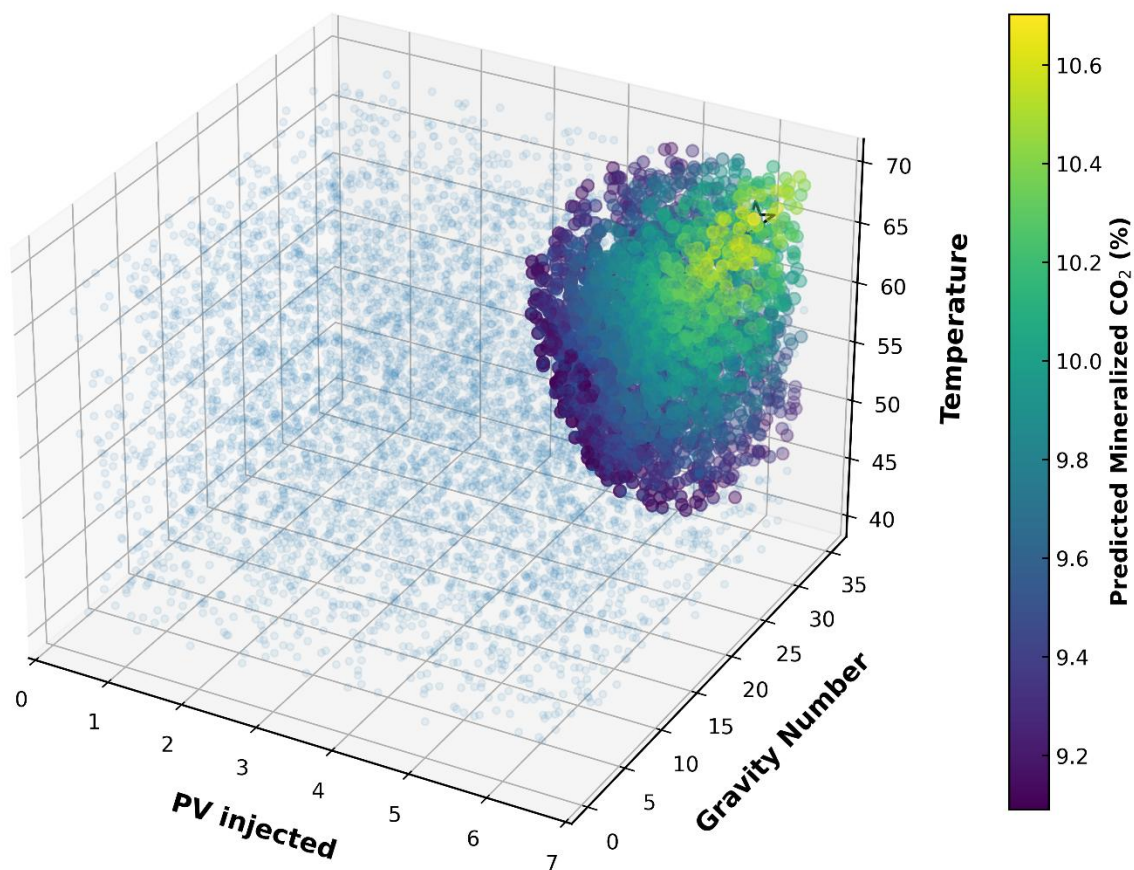


Figure 25. Three-dimensional inverse-design response space for mineralized CO₂ fraction under conservative conditions. All input parameters except PV injected (Qd), Gravity Number, and temperature were fixed at their 5th percentile values, while time was fixed at 200 years

5. CONCLUSION AND RECOMMENDATIONS

This study developed a physics-guided machine-learning framework to predict the temporal evolution of CO₂ trapping mechanisms in heterogeneous deep saline aquifers. By combining long-term compositional reactive-transport simulations with data-driven surrogate models, the study addressed the high computational cost of repeated full-physics simulation. Adopted approach preserves physical relevance through dimensionless and mechanism-oriented input variables. The results demonstrated that the proposed framework can accurately predict supercritical, dissolved, residually trapped, and mineralized CO₂ fractions over time, and can further be used for inverse design aimed to enhance long-term storage security.

The main conclusions of this study are as follows:

1. TabM showed the best and most stable predictive performance among the tested models. Across the train, test, and 5-fold cross-validation results, TabM consistently achieved the highest predictive accuracy for all four trapping mechanisms. It outperformed CatBoost, FTTransformer, LightGBM, XGBoost, Random Forest, Symbolic Regression, and the baseline models. In particular, the baseline models Decision Tree and Linear Regression showed the weakest overall predictive capability, which confirms that simple model structures are insufficient to capture the nonlinear and coupled controls that govern long-term CO₂ trapping. Tree-based methods provided superior performance compared with the baseline models, whereas TabM showed the best overall balance of accuracy, robustness, and generalization.
2. The governing controls are different for different trapping mechanisms. The feature-importance analysis showed that the most influential variables are not the same for the four trapping mechanisms. For supercritical and dissolved CO₂, the dominant factors are elapsed time, salinity, gravity number, and PV injected, while for residual trapping residual gas saturation is the dominant parameter, consistent with the strong dependence of hysteresis trapping. For mineral trapping, the most influential inputs are elapsed time, PV injected, gravity number, and temperature.
3. The developed framework provides a fast and practical additional tool that can be used for pre-screening before repeated full-physics simulation. Once trained, the surrogate models can evaluate large numbers of scenarios in seconds. This makes the framework suitable for screening, sensitivity analysis, uncertainty evaluation, and optimization.

The speed advantage is especially important for inverse design, where a large design space must be explored efficiently. In this study, the trained model was successfully used to identify the parameter ranges associated with the most highly mineralized cases.

4. Inverse design provides actionable guidance for improving long-term mineral trapping. The inverse optimization analysis showed that enhanced mineralization is associated with a balanced operating window rather than extreme values of individual parameters. The most favorable cases clustered within relatively narrow percentile ranges of the governing variables. This indicates that long-term mineral trapping is promoted by a combined effect of sufficiently strong injection, moderate drawdown, moderate heterogeneity, controlled residual gas saturation, and favorable thermodynamic conditions. The favorable ranges identified from the optimal cases were $Q_d = 4.72\text{--}6.12$, dimensionless drawdown = $0.64\text{--}1.07$, $VDP = 0.26\text{--}0.65$, $S_{gr} = 0.15\text{--}0.30$, gravity number = $18.14\text{--}28.80$, temperature = $55.18\text{--}65.67\text{ }^{\circ}\text{C}$, and salinity = $3.00\text{--}4.54$ M. These results suggest that such percentile-based intervals may be used as preliminary screening guidelines for identifying candidate reservoirs and narrowing operational scenarios before computationally intensive full-physics simulations.

Overall, this study confirms that physics-guided machine learning can serve as an efficient and interpretable surrogate for modeling long-term CO_2 trapping in saline aquifers. The results further indicate that dissolved and residual trapping contribute strongly to long-term storage, whereas mineral trapping develops more gradually and therefore requires longer evaluation times to be properly assessed. By the combination of predictive accuracy, physical interpretability, and computational efficiency, the proposed framework offers a promising tool for CCS assessment and design.

Based on these findings, several recommendations can be made. For mineral-trapping-oriented CO_2 storage assessment, reservoir screening should not focus on maximizing any single variable independently. Rather, it should aim to identify a balanced parameters window. Therefore, the optimal percentile ranges identified in this study may serve as practical first-pass screening criteria for selecting candidate reservoirs and defining promising operating conditions for more detailed investigation.

At the same time, the current framework should be interpreted within the limits of the simulation dataset used for training. Although geological heterogeneity was included, the framework does not explicitly account for more complex structural features such as faults,

fractures, or strong compartmentalization, all of which may significantly influence CO₂ migration and trapping behavior. In addition, the input parameters were sampled from independent uniform distributions, which neglect natural geological correlations, such as those between depth and temperature or between porosity and permeability. Reactive-transport kinetics and relative-permeability relationships were also adopted from generic literature values rather than field-specific laboratory or site measurements. Furthermore, geomechanical effects, wellbore integrity, and injection-induced stress changes were outside the scope of the present compositional modeling framework. Finally, the developed surrogate models were validated only against synthetic simulation data, and therefore their predictive robustness under real field conditions remains to be confirmed.

Accordingly, future work should focus on improvement of both physical realism and the generalizability of the proposed framework. One important direction is the inclusion of more advanced heterogeneity parameters, such as correlation lengths, anisotropy measures, facies connectivity, layering contrast and other related parameters. The incorporation of more geologically realistic reservoir architectures, which include faults and fractures, would further improve applicability to field-scale systems. Coupling the framework with geomechanical simulation would allow evaluation of injection-induced stress changes and caprock integrity risks. Most importantly, the surrogate models should be validated against the independent datasets, pilot-scale observations, or blind field tests to confirm their predictive robustness outside the synthetic design space considered in this study. These improvements would strengthen the framework as a reliable decision-support tool for long-term CO₂ storage design and optimization.

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