

Article

Numerical Reservoir Simulation of CO₂ Storage in Saline Aquifers: Assessment of Trapping Mechanisms, Geochemistry, O₂ Impurities and Brine Salinity

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Abstract

It is a challenge in experimental studies today to accurately predict the trapping mechanisms in saline aquifers that influence the long-term CO₂ storage capacities. The inability in current experimental studies to quantify the effects of combined processes of solubility, hysteresis, and mineralization as a means of affecting saline aquifer properties that influence CO₂ trapping mechanisms makes this topic interesting. A systematic framework in CMG-GEM compositional simulation studies is proposed in this article to assess the effects of gradually modelled trapping mechanisms on CO₂ storage performance. Simulation studies are conducted under identical constraints, trapping mechanisms, as well as operational factors in a sequential process that activates (i) solubility, (ii) solubility + hysteresis, and (iii) solubility + hysteresis + mineralization. The findings demonstrate distinct differences in trapping process behaviors as well as simulation stability under various modes: hysteresis effects largely improve immobile reserves as well as decrease plume migration, and, on the other hand, mineralization adds long-term dynamics of capacity increase as well as porosity-permeability alterations, especially in carbonate reservoirs. Through long-term post-injection simulations (up to 1000 years), the findings demonstrate that various trapping processes trigger over distinct time periods—years for immobile reserves, decades for dissolution, and centuries in the case of mineralization. This contribution is able to point out the computational efficiency as well as defective model behavior of concern to various physics levels, providing a practical guide to modelers in making a well-informed decision on what constitutes a minimum set of physics in long-term trustworthy CO₂ storage.

Keywords: reservoir simulation; CO₂ storage; saline Aquifers; CO₂ trapping mechanisms; geochemistry; brine salinity; CMG-GEM and O₂ impurities



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1. Introduction

Injecting carbon dioxide (CO₂) into deep saline reservoirs is well identified as a key solution in large-scale, long-term CO₂ capture. In spite of the positive results of pilot scale demonstrations of injection and trapping of CO₂, major uncertainties exist in simulating reservoir performance in terms of the absolute amount of CO₂ that is reliably trapped long-term, as well as in understanding the importance of various trapping mechanisms of CO₂. These uncertainties exist mainly because of simplifications in the reservoir simulation model, especially due to the absence of certain trapping mechanisms [1–3].

Until now, numerical analysis has routinely been conducted either around a single trapping process or a type of rock, ignoring the combined effects of various physics in the

same boundary condition settings. In fact, not much consideration has been given in the literature to the numerical aspects of employing advanced capabilities in commercial codes like hysteresis or reacting transport. Therefore, there is no general framework in this field that presents, in a quantitative way, when a set of physics affects results in a practical way and when a simpler model is sufficient [4–7].

This research bridges this gap by carrying out a comparative simulation analysis of CMG-GEM applied to a base model with simplified representation then incorporating the different trapping mechanisms, and finally applying this to two different geological settings (Clastic & Carbonate aquifers) [7–9].

Simulation time is increased to 1000 years to capture long-term transitions between the various trapping schemes and assess when a particular scheme becomes dominant. Various model results, including those involving CO₂ molality, reduction in porosity as well as permeability, as well as mass balance convergence, are investigated in order to gauge the realism of model parameterization.

This is a rigorous comparative analysis of physics modes, rock properties, and long-term trapping mechanics that has been done in a unified numerical framework. In particular, this is not a parameter scan-based analysis where a machine learning model is used as a surrogate to predict the results, but rather a physics-informed diagnostic analysis that will point out the trapping processes that are mandatory in a trustworthy CCS simulation model, as well as those that could cause unwanted model complexity [3,6].

2. Literature Review

Carbon Capture, Utilization, and Storage (CCUS) is identified as one of the most effective solutions to curb human-made CO₂ emissions in achieving a net-zero energy sector. Compared to various possible sites in geologic storage, Deep Saline Aquifers (DSAs) offer the greatest worldwide penetration due to their extensive geographical coverage, high porosity-permeability properties, as well as separation from the Earth's surface by overlying layers of caprock [8–10]. Injected CO₂ in DSAs is trapped through a range of mechanisms such as structural, residual, solubility, as well as mineral spanning various time-scales [7–10]. Structural trapping is primarily accountable for short-term residence time of CO₂, as opposed to long-term trapping via solubility and mineral mechanisms spanning tens of thousands of years [11,12].

2.1. Geological Controls and Flow Behavior

Geological controls strongly influence the flow behavior and distribution of CO₂ within subsurface storage formations such as saline aquifers and depleted hydrocarbon reservoirs. Key geological factors—including rock type, depositional environment, facies distribution, structural setting, porosity–permeability variations, fractures, and caprock integrity—govern how CO₂ moves, spreads, and becomes trapped within the reservoir. Reservoir heterogeneity, particularly common in complex systems, creates preferential flow pathways and uneven plume migration. High-permeability zones, channels, or fracture networks can accelerate CO₂ movement, while low-permeability barriers or baffles may restrict flow and lead to localized accumulation. These geological structures strongly impact injectivity, sweep efficiency, storage capacity, and pressure distribution during and after injection [10–14].

The flow behavior of injected CO₂ is also controlled by fluid and rock properties, including density contrast, viscosity ratio, capillary forces, and wettability. Supercritical CO₂ is less dense and less viscous than brine, causing it to migrate upward due to buoyancy, especially when vertical permeability and structural dip are high. Capillary pressure and wettability determine how easily CO₂ can displace brine and how much remains immobile

through residual trapping. In strongly water-wet reservoirs, capillary forces resist CO₂ invasion into smaller pore spaces, enhancing immobilization but potentially reducing injectivity. Geological controls also determine the effectiveness of trapping mechanisms such as structural, residual, solubility, and mineral trapping, which together influence long-term storage security [12–15].

Understanding these geological factors is essential for building accurate reservoir models and simulation strategies, enabling prediction of plume evolution and identification of potential leakage pathways. Integrated analysis through seismic interpretation, core studies, well logs, and dynamic production or injection data is crucial to characterize heterogeneity and guide injection design. Ultimately, successful CCS projects rely on accurately assessing geological controls to ensure efficient flow behavior, stable storage, and safe long-term containment of CO₂ [10,12].

Heterogeneities in the reservoir play a critical role in CO₂ migration and entrapment. The Sequential Gaussian Simulation was employed to assess the influence of correlation length and permeability variance on the morphology of CO₂ migration in a heterogeneous reservoir [15]. The results revealed four flow regimes, including a dispersive, sweeping, fingering, and channeling flow regime, where intermediate values of heterogeneity promote CO₂ dissolution and trapping.

Based on a conducted history-match modeling process, over a period of 100 years, the Sleipner field will see a transition from structural trapping to solubility-trapping, followed by a substantial contribution of mineralization as a trapping mechanism [9,16–18].

2.2. Geochemical and Mineral Trapping

Injected CO₂, brine, as well as rock minerals' reactions are particularly important in long-term as solubility trapping and residual trapping are mutually enhancing; initial water saturation assists in trapped gas dissolution. Also, it was observed that in the case of sandstone aquifers with a small quantity of reactive minerals, the process of mineralization is negligible over a period of 500 years, signifying that solubility and hysteresis effects are dominant under normal conditions [8,19].

3. Methodology and Workflow Integration

The most adaptive management approach is one that emphasizes the principle of 'fit for purpose' models that match the phase of a project, data availability, and regulatory needs.

3.1. Model Extent and Grid Cell Dimensions

In numerical reservoir simulation, the extent of the model is essentially a means of defining the horizontal and vertical dimensions of a domain that can be used to realistically model the storage formation, the overburden, and possibly underlying units [20]. The horizontal extent of a model is usually selected to accommodate the full range of CO₂ plume migration, pressure, and boundary effects that need consideration over the duration of a simulation, without unnecessarily extending a model's dimensions and hence its computation time [10,20]. Vertically, a typical model or reservoir simulation may include the reservoir interval of interests, key baffles or high permeability layers within reservoirs, the main caprock, and, if necessary, a lower or secondary seal or aquitard. It is necessary that its boundaries be far enough from areas of CO₂ and pressure behavior of interests to be independent of the boundaries [21].

The size of the grid cells controls the spatial accuracy of a simulation. Although a smaller cell size offers a better description of variability, transition zones, wellbore proximity, and saturation or pressure-front positions, larger numbers of dimensions increase

computation time and require smaller time step sizes [19–22]. Larger grid sizes result in larger numerical effort but reduce simulations' accuracy of important processes such as capillary trapping or fingering. The strategy is to increase grid size around wellbore and areas where strong spatial changes can be anticipated, for example, around the injection zone and high-flow zones, and to decrease grid size towards a larger domain. Note that the dimension of a grid model cell must be capable of honoring the reservoir's spatial variability, as well as the spatial variability of its confining layers. Inadequate sizes of a grid dimension can cause numerical dispersion, saturation errors, and sensitivity of a grid size, as suggested by [20–25].

3.2. Data Integration and Uncertainty Analysis

Data integration and uncertainty evaluation form basic parts of sound reservoir characterization and forecasting for CO₂ storage. The natural complexity of geological systems, combined with limited and non-uniform data, makes data integration a powerful tool for comprehensive reservoir characterization and a better-informed forecasting of CO₂ cloud transport, injectivity, pressure, and long-term storage security. Basic data to be integrated include geological, geophysical, petrophysical, geochemical, and dynamic reservoir data such as core and SCAL data, well logging, seismic interpretation, pressure and rate history, and geochemical analyses. By combining these through multidisciplinary interpretations and comparisons, a better-informed, more realistic reservoir model can be developed that realistically represents the natural complexity of the reservoir [22–26].

Uncertainty analysis is a method to quantify the possible range of model outcomes that arise for reasons of incomplete reservoir knowledge, errors of measurement, simplified model assumptions, and variability of key parameters such as permeability, porosity, capillary pressure, relative permeability, geochemical reaction constants, and boundary conditions. It is done through sensitivity analyses, probabilistic simulations, and scenario testing, where a number of realizations of a reservoir model can be generated by using different parameter combinations for uncertain parameters. Monte Carlo simulation, experimental design, geological stochastic models, and ensemble-based methods of model adaptation can be applied to obtain a better estimation of uncertainties, being most sensitive to reservoir parameters that influence CO₂ storage [24,26–28].

Data and uncertainty evaluation integration are key tools to inform risk management, decision-making, and system design for optimal injection, monitoring, and regulatory compliance. By grasping the 'uncertainty envelope' rather than a 'single deterministic result', a better CCS evaluation on storage capacity, leakage risk, and feasibility can be obtained. Data evaluation for a CCS effort, as stated, is improved by a thorough uncertainty evaluation. It's recommended a sequence of 'stochastic realizations to quantify uncertainties of structure and properties [25–27].

3.3. Simulation Design

Simulation design is a process of systematically laying out a plan for constructing a numerical reservoir model to assess CO₂ injection, plume transport, and storage security. Efficient simulation designs also make sure that a numerical reservoir model is able to properly describe the geological system. The simulation design starts by determining what the objectives of the simulation task or problem are. These objectives include evaluating trapping efficiency, testing injection capacity, determining the transport of a plume, evaluating methods of pressure management, or evaluating capacity for storage. These objectives determine the design of a numerical reservoir model that requires assumptions, processes, boundaries, or data [27–30].

Good simulation design involves choosing a suitable grid size, dimensions, numerical solver, and fluid equations. It is necessary to determine if a fully compositional simulator is required, capable of addressing processes such as dissolution, density-driven convection, and geochemical reaction, or a black oil or simplified simulator, if less complex. Based on the selected simulation design, a numerical model is developed to incorporate initial and boundary conditions, such as reservoir pressure, temperature, saturations, and capillary pressure. Finally, injection parameters, such as injection rate, injection location, intervals for injection, and duration of injection, can be incorporated to replicate possible injection schemes [30–33].

Simulation design incorporates trapping processes such as structural, residual, solubility, and mineral trapping, coupling relative permeability hysteresis, geochemical processes, and pressure decay. Sensitivity to key parameters such as permeability, porosity, wettability, capillary pressure curves, geochemical kinetics, fault transmissibility, and heterogeneity is incorporated from the outset to assess uncertainties. Calibration techniques via history matching, if dynamic data is available, can increase the validity of the simulation, and scenario methods test different injection and monitoring designs [31–36].

Ultimately, a balanced simulation design, incorporating geological realism, process realism, and computer capabilities, offers a powerful tool for reservoir performance prediction, safer and more efficient CO₂ injection, or monitoring of CO₂ injection processes [35].

Hysteresis effects for relative permeability, capillary pressure curves, and primary trapping must be incorporated into simulation models. Moreover, incorporating the caprock into a simulation model makes possible the evaluation of the efficacy of brine trapping [29].

3.4. Dynamic Updating

The dynamic updating aspect is a vital step in reservoir simulation and management for CO₂ injection projects, enabling the simulation model to develop and be refined by available new data from the reservoir. Given that geological properties and injection behavior are uncertain, projections developed prior to injection can be different from what happens in a reservoir. The dynamic updating process continually feeds data from monitoring, such as pressure, rate of injection, fluid properties, plume mapping data such as seismic, and well injection performance to the simulation model to enable accurate representation of actual behavior of a reservoir [25–27].

Over a long period of monitoring, the model is updated multiple times, each of these attempts improving the knowledge of pressure propagation, plume evolution, and trapping processes. The dynamic updating of the model assists in making better decisions through testing different assumptions for a scenario, changing injection rates, shifting injection locations, or carrying out different methods of pressure management, such as water injection or two-well injection optimization. It can also be used for regulatory compliance and validation to ensure that the storage process is safe and performs within its required capacity. Essentially, dynamic updating of the reservoir model makes a predictive system that was static a dynamic entity, making CO₂ storage a much safer operation [32–35].

3.5. Large-Scale and Long-Term Modeling

Large-scale and long-term models of the system are required for the forecast of behavior and/or long-term performance of CO₂ storage projects extending from decades to thousands of years after injection, far beyond the actual injection horizon. In contradistinction to short-term models, largely constricted to spatial and temporal scales of injectivity and short-term near-injection-site behavior, full-scale models of CO₂ transport and trapping take into consideration the entire spatial domain of a plume or of regional pressure propa-

gation, along with trapping processes that evolve within a reservoir. These models require a high degree of geological detail, including regional geometrical trends, fault systems, and multiple geological units. They serve to ensure that interaction between injection points or reservoirs and the geology of the larger world is adequately modeled, especially for establishing regional pressure distributions [24,31].

Additionally, long-term models incorporate multiphase flow, geochemical processes, and trapping for the simulation of post-injection CO₂ storage processes. Over geological time, CO₂ processes include the structural, residual, solubility, and mineral trapping phases, all of which affect storage security and CO₂ plume migration. Numerical stability, strong geochemical coupling, and a representation of relative permeability hysteretic behavior, along with dynamic capillary pressure, must be incorporated to determine the long-term entrapment of CO₂. Simulation of CO₂ pressure dissipation along leakage boundaries, due to brine displacement or managed CO₂ storage plan through methods, such as the extraction of formation brine, is of high importance for regional simulations [15,18,22].

Owing to the uncertainties associated with long-term CO₂ storage simulation, these codes can be alternatively applied to different simulation conditions to test a number of possible future outcomes and risks associated with fault reactivation, seal capacity of the caprock, and possible leakage paths. Based on long-term simulations, CCS can provide scientific validation to ensure that CO₂ injected into underground reservoirs is safely trapped for thousands of years [12,21].

In addition, the influence of inter-intervals of shale, as well as faulting, was analyzed on the CO₂ injection process and outputs concluded that a high value of heterogeneity leads to a localized accumulation of CO₂, but its rate of dissolution is lessened [16–19].

3.6. Workflow and Simulation Setup

A sequential modeling process has been developed to model the entire chain of CO₂ storage processes in a deep saline reservoir, starting from fluid properties to compositional simulation modeling, as well as post-processing of trapping data [32]. This process is divided into four main steps:

3.6.1. PVT and EOS Definition

Pressure-Volume-Temperature (PVT) behavior refers to the fluid properties of CO₂, brine, oil, and gas at subsurface conditions of varying pressure and temperature. PVT behavior is a crucial aspect of CO₂ storage and enhanced recovery, as CO₂, a substance that is mostly composed of CO₂, changes phase according to the temperature and pressure of its location. Below the critical temperature and pressure of 31.1 °C and 7.38 MPa, CO₂ is a gas, but above these conditions, CO₂ is a supercritical fluid that possesses high density, typical of a liquid, and low viscosity, typical of a gas. This makes it possible for a supercritical fluid to move through a porous medium and occupy a considerable mass of space [34–36].

An Equation of State (EOS) is a mathematical representation of the relationships among pressure, temperature, and volume of a fluid system that exists in multiple phases. The PR-EOS or SRK models of EOS are applied to CO₂ for numerical simulation of its behavior. These models describe CO₂ interaction processes with different components, such as water, other components of natural gas, and impurities [37,38]. These processes include interaction of CO₂ with components such as water, hydrocarbons, and impurities such as nitrogen, sulfur dioxide, hydrogen sulfide. These models of EOS are integrated into reservoir models, where CO₂ injection processes for CCS can be simulated [35–37].

PVT analysis and EOS simulation combined provide a basis for injection strategy design, parameters optimization, estimation of efficient storage, and evaluation of possible risks, such as pressure increase or problems of caprock integrity. Without a detailed

description of PVT and EOS, reservoir simulation could give incorrect results, making these techniques vital to successful CCS development [37–39].

This specific research is a follow-up of a larger case study review that is centered on the topic of subsurface fluid modelling for carbon capture and storage (CCS), where the significance of a subsurface fluid characterization that suitably affects the reservoir simulation result is highlighted. In this context, the CMG-WinProp model for PVT & EOS is most appropriate for simulating the phase properties of CO₂-brine. Underlying is the given procedure [33,35].

Component Characterization

Component characterization is a basic step of compositional reservoir simulation for CO₂ storage. It is a description of all fluid components available within a system and their interaction. In a CO₂ storage system, for example, CO₂ is a main system component. Moreover, other components that can be found within a formation fluid include water and salts, such as NaCl. These components make up a system of a CO₂ storage process.

Equation-of-State Tuning

Equation of State (EOS) matching is a key step for compositional reservoir simulation to ensure that the choice of EOS can match the experimental PVT data of the existing fluid components in the system. In CO₂ storage simulation, the Peng-Robinson Equation of State (PR-EOS) is preferred because of its ability to describe the behavior of non-polar to moderately polar components, especially around the critical region of CO₂.

The tuned EOS is the basis of a compositional simulation package, enabling accurate representations of thermo-dynamics to facilitate the simulation of two-phase flow, trapping, and geochemical processes. The objective of this step is to ensure that the simulation process is able to predict the actual behavior of the reservoir [38,39].

Phase-Equilibrium Validation

Validation of phase equilibrium plays a vital role in compositional modeling to confirm that a pertinent and matched Equation of State is able to represent the actual phase behavior of CO₂-brine systems. In the context of CO₂ geological storage, the phase behavior of supercritical CO₂ and formation-brine interaction plays a key role in determining the rate of dissolution, solubility trapping, density, and CO₂ plume migration. Validation of the equation of state was performed, incorporating experimental validation of phase behavior, phase equilibrium, CO₂ solubility, and the transition from a one-phase to a two-phase region.

The parametrically tuned EOS was able to simulate the solubility of CO₂ properly in formation brine, ensuring that CO₂ was modeled to dissolve properly as a result of its dependence on pressure, temperature, and concentration. Furthermore, the phase boundaries that separate gaseous, supercritical, and dissolved CO₂ phases matched experimental vapor-liquid equilibrium data properly, enabling validation of transition points, thus ensuring that a real CO₂ density and viscosity range was obtained, especially for a working pressure range of 10–25 MPa, typical for deep aquifers that can be found for CCS. Density and viscosity of CO₂ affect directly buoyancy forces, plume shapes, injectivity behavior, and dissolution kinetics.

It ensures that the behavior of CO₂ is predicted on the basis of a sound and accurate platform that validates phase behavior and properties, thus offering a firm basis for simulating processes of two-phase flow, dissolution trapping, and evolution of long-term storage, since the next simulation stages are made possible through physically accurate thermodynamic performances.

Fluid-Model Export

After finishing the EOS tuning and validation of phase equilibria, the resulting fluid property package was exported directly from CMG-GEM for compositional reservoir simulation. By transferring the tuned component parameters, interaction parameters, and volume-translated parameters of the Peng-Robinson EOS to CMG-GEM, the simulation model is capable of simulating CO₂-brine processes such as the interaction of the phases, dissolution, density-driven convection, and long-term trapping for CO₂ injected into a geological formation [32,37].

By incorporating the customized fluid property package into the GEM, the simulator can determine accurate phase behavior, fluid density, viscosity, interfacial tension, and solubility dynamics for injection and storage. It is also capable of handling advanced geochemical coupling for mineral reaction processes or aqueous species. The direct export method eliminates the possibility of errors introduced through manual entry of parameters. This makes the compositional simulator module of GEM a capable tool for CO₂ plume migration, injectivity, pressure, and long-term CO₂ containment [36–39].

3.6.2. Reservoir Model Description and Boundary Conditions

The base modeled aquifer represents a deep confined formation with a depth of 1.4 km, initial pressure of 20 MPa, temperature of 50 °C, equivalent with reservoir grid comprises 100 × 100 × 30 cells. was located at grid block (1,1,1), which was perforated in the bottom three layers from 28 to 30 (highlighted in the red circle in Figure 1). The model's constraints were set at a maximum bottom hole pressure of 45,000 kPa and a maximum surface gas rate of 12,000 m³/day. Table 1 outlines the parameters for the base case of CO₂ injection into a saline aquifer, while Figure 1 displays the corresponding 3D model [40].

Table 1. Saline aquifer system input parameters [40].

Aquifer Parameters	Values
Grid number	300,000 (100 × 100 × 30)
Length (m)	1000
Width (m)	1000
Depth at the top (m)	1200
Thickness (m)	30
Permeability (md)	150
Porosity (%)	0.23
Salinity (M)	1.7
Component	CO ₂
Critical Pressure (atm)	72.8
Critical Temperature (C)	50

After the injection period, the well is shut-in, and the system is allowed to evolve naturally for an additional 199 years to capture long-term dissolution and mineral trapping.

Different total simulation times are tested 200, 500 and 1000 yrs, along with variable the end of Injection (EOI), ranges from 1 to 50 years

Furthermore, three progressive physics modes were simulated for each rock type to isolate the incremental influence of added processes:

Mode 1—Solubility only: physical dissolution of CO₂ in brine.

Mode 2—Solubility + Hysteresis: inclusion of relative-permeability and capillary-pressure hysteresis.

Mode 3—Solubility + Hysteresis + Mineralization: addition of geochemical reactions (kinetic rate law) representing mineral dissolution and carbonate precipitation.

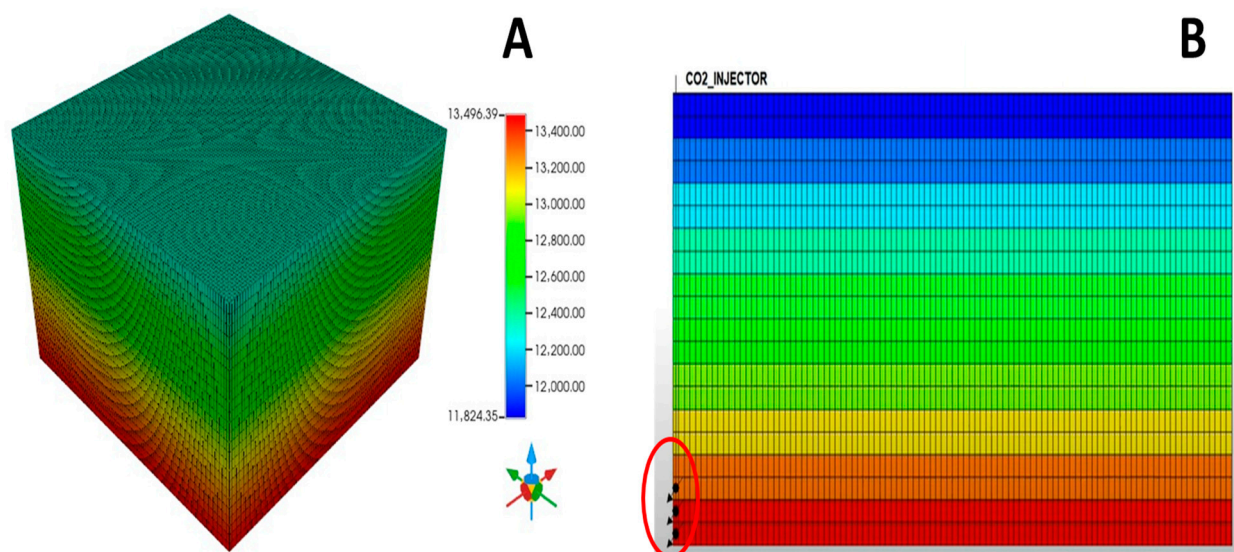


Figure 1. (A) Simulation model 3D view and (B) Simulation model side view [40].

3.6.3. Relative Permeability and Hysteresis

Relative permeability and hysteresis effects become extremely important for describing two-phase or multiphase flow processes occurring during CO₂ injection and storage processes within geological formations, such as saline aquifers and depleted reservoirs. When CO₂ is injected into a reservoir filled with a solution of brine, these two phases do not occupy the pore space simultaneously. Both phases occupy their own separate channels, and the movement of each fluid is measured by relative permeability, which is a property of fluid saturation. When the saturation of CO₂ increases, its relative permeability also increases, and the relative permeability of brine decreases as a result of displacement from the pore space [26–29].

Hysteresis is the difference of behavior of relative permeability for the injection (drainage) process and the post-injection process. When CO₂ is injected, CO₂ molecules replace the brine, moving to larger pores. After the injection is stopped, and as a result of capillary forces, the brine starts moving back into the reservoir. It creates a situation where CO₂ is isolated as ganglia from pore contacts, a situation known as trapping. Hysteresis, therefore, causes the relative permeability curve to differ for the imbibition and drainage processes. It affects the rate of increase of relative permeability of brine and the rate of decrease of relative permeability of CO₂. Hysteresis is another important CO₂ trapping mechanism that inhibits CO₂ migration to higher reservoirs, making storage safer [22,25–27].

Relative permeability and hysteresis properties play a key role for reservoir simulation, affecting CO₂ plume migration, storage, injectivity, and ultimate recharge. Relative permeability curves can be determined through core flood experiments, SCAL, and matched reservoir simulator results. These two properties behave differently for Clastic and carbonate reservoirs, depending on pore type, wettability, and capillary pressure. Relative permeability for the CO₂-H₂O system was evaluated using the Corey type correlation, tuning endpoints to match a standard correction curve. Hysteresis was turned on using a trapping coefficient value, $J = 0.2$ – 0.4 . Relative permeability of gas and hysteresis curves is depicted by Figures 2 and 3 respectively [26–28,40]. In Figure 2 the plot shows the relative permeability of gas in blue and relative permeability of water in red versus to the water

saturation while Figure 3 includes gas the sensitivity range of hysteresis coefficient values in different colors.

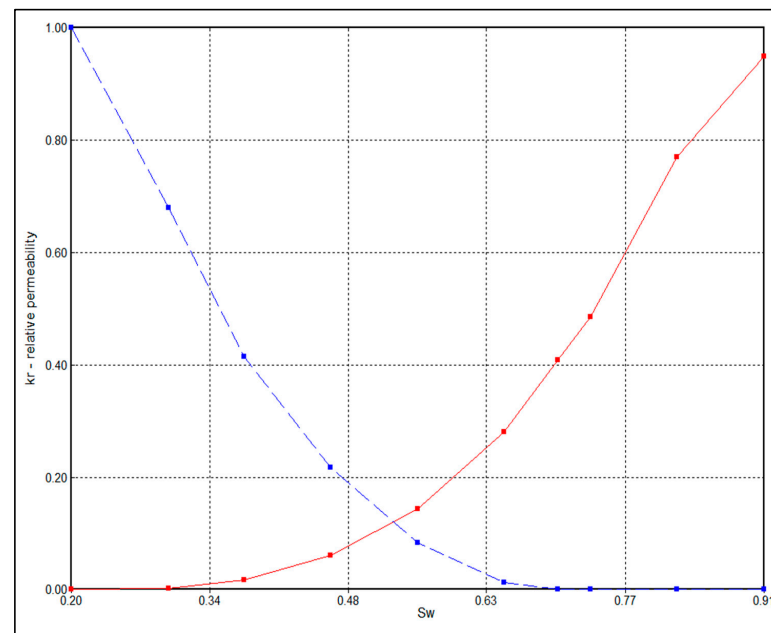


Figure 2. The Gas Relative Permeability Curve.

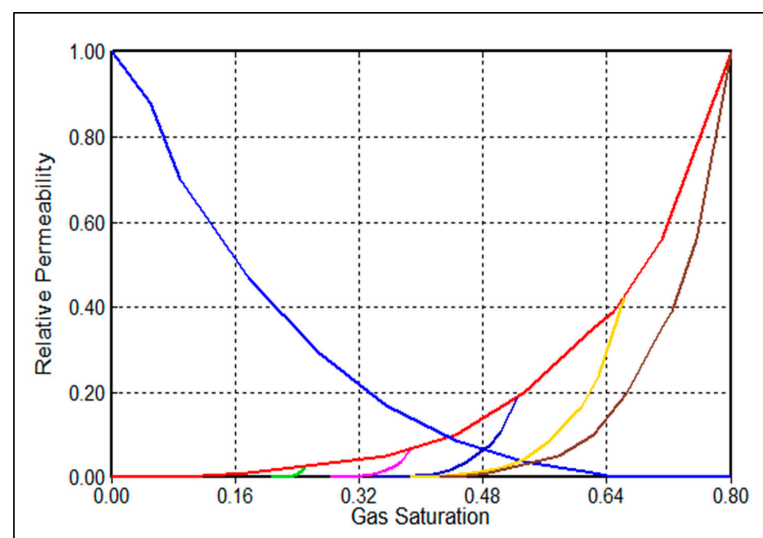


Figure 3. The different hysteresis Curves.

3.6.4. CO₂ Dissolution

CO₂ dissolution is a crucial process for the long-term storage of CO₂ in geological reservoirs and is a fundamental aspect of CO₂ storage for improving the security and stability of CCS. Once injected, the CO₂ is initially formed as a separate phase that is less dense than the formation brine, hence moving towards migration to the top of the reservoir. However, as time passes, the CO₂ dissolves in the formation brine through diffusion and convective transport. When CO₂ combines with water, a weak acid called carbonic acid is produced, resulting in a decrease in the pH of the formation brine. Once dissolved, the density of CO₂ becomes greater than that of the formation brine, hence sinking through the reservoir due to convective dissolution or density-driven convection [35–37].

The process of dissolution is much better for storage security because the CO₂ that is dissolved is neither able to migrate nor form a plume. Dissolved CO₂ causes the onset of

geochemical reactions along with minerals from the reservoir, possibly forming a long-term trap through the precipitation of carbonate minerals. The rate of dissolution of CO₂ is a function of a range of parameters, such as temperature, pressure, salinity, and formation and fluid properties. Higher pressure and lower salinity velocities increase the solubility of CO₂, although heterogeneity may favor or suppress patterns of interaction. Dissolution is regarded as a prominent trapping method for periods measured from decades to centuries for many aquifers [29–31].

In summary, CO₂ dissolution is a key mediating step between the processes of structural/residual trapping and mineral trapping, offering a safe route for CO₂ storage. It is a process that assists in stabilizing the plume and reduces the need for its physical trapping.

3.6.5. Aqueous and Mineral Reactions

Aqueous and mineral reactions can have a vital role in the long-term fate and security of CO₂ geological storage. When CO₂ is injected into a subsurface reservoir, CO₂ dissolves into the formation-brine solution, forming H₂CO₃, or carbonic acid, and leading to a decrease in pH, making the pore-water solution highly acidic. The high acidity supports aqueous reactions for CO₂-rich brine and reservoir minerals. At first, when the acidic fluid comes into contact with these minerals, carbonates and silicates react, releasing Ca²⁺, Mg²⁺, Fe²⁺, and Na⁺ ions into the solution. This reaction can increase porosity and permeability, making CO₂ injection easier [18–20].

When these ions build up, the system gradually readjusts, making way for the precipitation of secondary minerals. These precipitation reactions can result in the entrapment of stable carbonate minerals like calcite, dolomite, magnesite, or siderite, depending on the original mineralogy of the reservoir. This is a crucial step for mineral trapping, within which CO₂ is irreversibly trapped as solid minerals. This is the most stable trapping mechanism, where CO₂ is trapped for the greatest duration. However, precipitation can also cause a decrease in permeability at the injection site or along fractures [9–11].

Water and mineral reactions depend on parameters such as temperature, pressure, salinity of the brine, pH, mineral composition, injection method, and properties of the CO₂ stream, such as SO₂, O₂, H₂S, etc. These components can increase the number of acid components and lead to changes in redox, among other factors. It is, therefore, vital to comprehend these reactions for forecasting geochemical evolution, porosity, reservoir capacity, and security of CO₂ storage [12–14].

A 3D model of a saline aquifer was generated using CMG-Builder. Grid sizes, as well as various matrices (porosity, permeability, thickness, etc.), were selected to encompass realistic storage formations, and all models had the same geometry. Three models of different frameworks were introduced.

Clastics

Clastic reservoirs can be defined as a type of reservoir that is filled with hydrocarbons, belonging to the group of clastic sedimentary rocks such as sandstone, siltstone, and sometimes conglomerates, generated as a result of the physical weathering and breakdown of rock fragments through erosion, transport, and deposition. These materials can be transported through river currents, glacial ice, or waves, as well as through air or ocean currents, and finally deposited at different sites such as fluvial channels, deltas, or deserts. After a long time, these materials get transformed into solid rock [41,42].

One of the most important characteristics of a clastic reservoir is that its porosity and permeability depend largely on grain size, sorting, cement, and packing. Compared to a carbonate reservoir, a reservoir's properties can be much more homogeneous, regular, and connected, since grains of sediment can be carried and placed according to a regular

stratigraphic trend. Most of the porosity of a clastic reservoir is intergranular, meaning that fluid flow is relatively easy. This is because a clastic reservoir is a single porosity reservoir [42].

Diagenesis remains relevant for a clastic reservoir, where reservoir properties can be altered by cementation of quartz or calcite, compaction, dissolution, or alteration of clay minerals. Over-cementation or the precipitation of clay minerals can lead to a reduction in permeability, whereas the dissolution of unstable minerals can increase pore volume. In such a situation, a clastic reservoir can form a tight gas reservoir, where fracturing is required to provide stimulation for enhanced output [41].

Industrially, Clastic Reservoirs can be found extensively all over the world; for example, deep-water turbidites, deltaic deposits, and fluvial channels. These reservoirs can be accessed quite conveniently, even without the same expertise required to tap carbonate reservoirs. Additionally, methods for enhanced oil recovery, such as ‘polymer flooding’ and ‘surfactants’, can be applied. They can be modeled for reservoir simulation, unconventional reserves, and CO₂ geological storage because of their predictability [41–44].

Overall, a clastic reservoir is more desirable than a carbonate reservoir because of its positive production behavior, simpler geological modeling, and homogeneous behavior of the reservoir, although challenges such as fines migration, clay swelling, and heterogeneity are also involved.

The reactive mineral system was modeled using calcite, kaolinite, anorthite, and halite, along with core carbonate aqueous reactions. Tables 2–4 shows the CO₂-brine interactions for elastic reservoirs bearing clay minerals and feldspar, along with initial concentration of aqueous species [39,42].

Table 2. Clastics Aqueous Reactions Selected [39].

No	Reaction	Function
1	$\text{CO}_2 + \text{H}_2\text{O} \leftrightarrow \text{H}^+ + \text{HCO}_3^-$	CO ₂ dissolution & acid formation
2	$\text{H}^+ + \text{OH}^- \leftrightarrow \text{H}_2\text{O}$	Water self-ionization
3	$\text{CO}_3^{2-} + \text{H}^+ \leftrightarrow \text{HCO}_3^-$	Carbonate equilibrium
4	$\text{CaOH}^+ + \text{H}^+ \leftrightarrow \text{Ca}^{2+} + \text{H}_2\text{O}$	Ca buffering from Ca-bearing minerals

Table 3. Clastics Minerals and Their Dissolution Reactions [39].

Mineral	Reaction	Significance
Calcite (CaCO ₃)	$\text{CaCO}_3 + \text{H}^+ \leftrightarrow \text{Ca}^{2+} + \text{HCO}_3^-$	Carbonate dissolution & pH buffering
Kaolinite (Al ₂ Si ₂ O ₅ (OH) ₄)	$(\text{Al}_2\text{Si}_2\text{O}_5(\text{OH})_4) + \text{H}^+ \rightarrow \text{Al}^{3+} + \text{SiO}_2 + \text{H}_2\text{O}$	Clay dissolution, releases Al & Si
Anorthite (CaAl ₂ Si ₂ O ₈)	$(\text{CaAl}_2\text{Si}_2\text{O}_8) + \text{H}^+ \rightarrow \text{Ca}^{2+} + \text{Al}^{3+} + \text{SiO}_2 + \text{H}_2\text{O}$	Feldspar dissolution, long-term reactivity
Halite (NaCl)	$\text{NaCl} \leftrightarrow \text{Na}^+ + \text{Cl}^-$	Controls salinity

Table 4. Initial Clastics Aqueous Species Values.

Species	Value (ppm)	What It Represents
pH	6.0	Slightly acidic starting fluid
Ca ²⁺	4999.98	Tied to calcite/anorthite dissolution
Na ⁺	90,000.1	High-salinity brine baseline
Al ³⁺	1 ppm	Seed concentration for aluminosilicate chemistry
SiO ₂ (aq)	181.089 ppm	Represents dissolved silica in brine
Cl [−]	1000 ppm	Balancing anion with Na ⁺

Calcite controls early pH buffering, while slower dissolution of kaolinite and anorthite influences long-term porosity evolution and secondary mineral formation.

Carbonates

Carbonates rank among the most prominent reservoirs of hydrocarbons worldwide, accumulating above 50–60% of the world's oil and gas reserves, especially in areas such as the Middle East, Northern Africa, and parts of North America. These reservoirs mainly result from the presence of carbonate rocks such as limestone and dolomite, which form due to biological and chemical activities that take place in shallow, tropical, and warm marine environments. As a result of the formation of most of these reservoirs from existing carbonate rocks, the environment of deposition for these reservoirs is quite heterogeneous [44–46].

One of the most typical properties of carbonate reservoirs is the complexity of the pore system. In this case, while the porosity of a typical clastic reservoir is dominantly intergranular, carbonate reservoirs could be composed of a range of different pore types such as vuggy, moldic, intraparticle, intercrystallite, cavernous, and/or fractures. These pore systems can be either connected or isolated, creating dual or multiple porosity systems, where the matrix can be saturated and the fractures can be the main conduits for fluid transport [45–47].

Diagenesis is also a very important factor that affects the quality of a carbonate reservoir. Dolomitization, dissolution, cementation, compaction, recrystallization, and karstification can be positive or negative for porosity and permeability. Dolomitization, for instance, is a positive process that creates intercrystallite porosity, improving reservoir quality, whereas cementation may be negative because of a decline in pore space. Also, karstification, through caves and/or large vugs, can create highly prolific reservoirs but makes drilling and development even more difficult.

From a technical viewpoint, carbonate reservoirs need sophisticated technical solutions [46,47].

Water injection, miscible gas injection (CO_2 , N_2), and smart well completions can be effectively applied for enhanced recovery, although the efficiency of the process may be limited because of fractures. Owing to geological intricacies, detailed characterization of a carbonate reservoir is necessary, incorporating seismic data, petrophysical, and dynamic characterization [43,44].

In summary, the resource potential of carbonate reservoirs is enormous, but they require the most advanced methods of reservoir management, oil recovery, and geological knowledge. And, as the energy transition moves towards carbon management, carbonate reservoirs or systems are now emerging as key to CCUS, because of the mineral reactions that can permanently trap CO_2 [42,46].

This system is a carbonate-evaporite mineral system, a typical system found for a carbonate aquifer under CO_2 injection. The selected minerals react to the aqueous species through dissolution-precipitation reactions, hence of significance to porosity, permeability, pH changes, and CO_2 trapping. Below are Tables 5 and 6, representing the Aqueous & Mineral selected Reactions, and Table 7 representing the initial concentration of aqueous mineral & Water pH value [39].

Table 5. Carbonate Aqueous Reactions Selected [39].

No	Reaction	Function
1	$\text{CO}_2 + \text{H}_2\text{O} \leftrightarrow \text{H}^+ + \text{HCO}_3^-$	Carbonic acid formation which is a key for pH buffering and CO_2 dissolution.
2	$\text{H}^+ + \text{OH}^- \leftrightarrow \text{H}_2\text{O}$	Water dissociation equilibrium that maintains charge balance.
3	$\text{CO}_3^{2-} + \text{H}^+ \leftrightarrow \text{HCO}_3^-$	Carbonate–bicarbonate for buffering equilibrium
4	$\text{CaOH}^+ + \text{H}^+ \leftrightarrow \text{Ca}^{2+} + \text{H}_2\text{O}$	Hydrolysis of calcium species
5	$\text{CaSO}_4 \leftrightarrow \text{Ca}^{2+} + \text{SO}_4^{2-}$	Calcium sulfate (anhydrite/gypsum) represents dissolution/precipitation equilibrium
6	$\text{MgSO}_4 \leftrightarrow \text{Mg}^{2+} + \text{SO}_4^{2-}$	Magnesium sulfate equilibrium (linked to dolomite and Mg minerals).
7	$\text{HSO}_4^- \leftrightarrow \text{H}^+ + \text{SO}_4^{2-}$	Bisulfate–sulfate acid-base equilibrium

Table 6. Carbonate Minerals and Their Dissolution Reactions [39].

Mineral	Reaction	Notes
Calcite (CaCO_3)	$\text{CaCO}_3 + \text{H}^+ \leftrightarrow \text{Ca}^{2+} + \text{HCO}_3^-$	
Dolomite ($\text{CaMg}(\text{CO}_3)_2$)	$\text{CaMg}(\text{CO}_3)_2 + 2\text{H}^+ \leftrightarrow \text{Ca}^{2+} + 2\text{HCO}_3^- + \text{Mg}^{2+}$	Very slow kinetics relative to calcite
Anhydrite (CaSO_4)	$\text{CaSO}_4 \leftrightarrow \text{Ca}^{2+} + \text{SO}_4^{2-}$	Dissolves moderately
Halite (NaCl)	$\text{NaCl} \leftrightarrow \text{Na}^+ + \text{Cl}^-$	Fast dissolution which affects salinity

Table 7. Initial Carbonates Aqueous Species Values.

Species	Initial Concentration	Meaning/Role
pH	6.0	Slightly acidic starting formation water
Ca^{2+}	5000 ppm (~5 g/L)	High calcium brine typical in carbonate or evaporitic basins
Mg^{2+}	2500 ppm (~2.5 g/L)	Supports dolomite reactions & Mg buffering
Na^+	90,000 ppm (~90 g/L)	Very high salinity; for of deep saline aquifer brines
SO_4^{2-}	1000 ppm (~1 g/L)	Sulfate required for anhydrite dissolution and ionic balance
Cl^-	1000 ppm (1 g/L)	Helps balance Na^+ charge; contributes to salinity

O₂ Impurities

O₂ impurities within Carbon Capture and Storage (CCS) can be understood to denote the presence of oxygen along with the captured CO₂ that is stored underground. In general, the CO₂ that is captured is never of 100% purity, and this depends on the method of CO₂ capture, such as post-combustion, oxy-fuel, or pre-combustion, where the CO₂ can be accompanied by gases such as O₂, N₂, H₂O, SO_x, NO_x, H₂S, or CH₄. Of these, oxygen is a key species because of its ability to react chemically [48,49].

The presence of oxygen within the injected CO₂ can result in the corrosion of materials within the wellbore, especially when combined with formation water to form an acid. Corrosion of wellbore materials can be enhanced by the presence of oxygen within carbon-steel tubing and cemented wellbore materials. Additionally, materials that can withstand such conditions or inhibitors that can resist such corrosion can be required to retain well integrity. This is especially the case when formation water is combined with oxygen [48–50].

In the subsurface reservoir, O₂ impurities can affect geochemical reactions among CO₂, brine, and reservoir minerals. O₂ can affect the redox state, leading to the oxidation of reduced minerals such as FeS₂, FeCO₃, or other Fe-containing minerals. These processes can affect porosity and permeability through mineral dissolution or precipitation. For instance, the oxidation of FeS₂ can form H₂SO₄, contributing to the initial increase in

porosity through the dissolution of carbonate minerals, and eventually to a decrease in permeability through the precipitation of secondary minerals [48–50].

Biologically, oxygen can also stimulate microbial activities in the reservoir environment; this can result in the formation of biofilms, plugging, or gases such as H₂S, among others, depending on the type of microbe. For these reasons, a maximum impurity specification is frequently established by CCS projects to manage the concentration of O₂ content within CO₂ streams, typically ≤10–100 ppm. Minimizing the presence of oxygen is beneficial, especially for extending the life of subsurface CO₂ storage [48,50].

The complete Fe–S–CO₂ geochemical system is a redox-sensitive system that includes aqueous iron and sulfur species, as well as their corresponding solid phases such as pyrite, siderite, and hematite. These processes can be simulated to determine the competition between carbonate dissolution, sulfate interaction, and other processes such as the oxidation of pyrite, precipitation of siderite, etc. [39].

Below are Tables 8 and 9, representing the Aqueous & Mineral selected Reactions, and Table 10 representing the initial concentration of aqueous mineral & Water pH value [39].

Table 8. O₂ impurities Aqueous Reactions Selected [39].

No	Reaction	Function
1	$\text{CO}_2 + \text{H}_2\text{O} \leftrightarrow \text{H}^+ + \text{HCO}_3^-$	CO ₂ dissolution & acid generation
2	$\text{H}^+ + \text{OH}^- \leftrightarrow \text{H}_2\text{O}$	Water acid-base balance
3	$\text{CO}_3^{2-} + \text{H}^+ \leftrightarrow \text{HCO}_3^-$	Carbonate buffering
4	$\text{CaSO}_4 \leftrightarrow \text{Ca}^{2+} + \text{SO}_4^{2-}$	Sulfate equilibrium
5	$\text{MgSO}_4 \leftrightarrow \text{Mg}^{2+} + \text{SO}_4^{2-}$	Magnesium buffering
6	$\text{FeSO}_4 \leftrightarrow \text{Fe}^{2+} + \text{SO}_4^{2-}$	Source of Fe ²⁺ into brine
7	$\text{H}^+ + \text{S}^{2-} \leftrightarrow \text{HS}^-$	Sulfide stability under reducing conditions
8	$\text{Fe}^{3+} \leftrightarrow \text{Fe}^{2+} + 0.25 \text{O}_2$	Fe redox conversion
9	$\text{H}_2\text{S} + 2\text{O}_2 \leftrightarrow \text{H}^+ + \text{SO}_4^{2-}$	Oxidation of H ₂ S (sulfur redox pathway)

Table 9. O₂ impurities Minerals and Their Dissolution Reactions [39].

Mineral	Reaction	Notes
Calcite (CaCO ₃)	$\text{CaCO}_3 + \text{H}^+ \leftrightarrow \text{Ca}^{2+} + \text{HCO}_3^-$	Carbonate dissolution/precipitation
Halite (NaCl)	$\text{NaCl} \leftrightarrow \text{Na}^+ + \text{Cl}^-$	Controls salinity
Anhydrite (CaSO ₄)	$\text{CaSO}_4 \leftrightarrow \text{Ca}^{2+} + \text{SO}_4^{2-}$	Sulfate mineral reaction
Hematite (Fe ₂ O ₃)	$\text{Fe}_2\text{O}_3 + 6\text{H}^+ \leftrightarrow 2\text{Fe}^{3+} + 3\text{H}_2\text{O}$	Fe ³⁺ source/redox buffer (EQUIL reaction)
Pyrite (FeS ₂)	$\text{FeS}_2 + \text{H}_2\text{O} \leftrightarrow \text{Fe}^{2+} + 1.75\text{HS}^- + 0.25\text{SO}_4^{2-}$	Sulfide mineral redox, acid generation
Siderite (FeCO ₃)	$\text{FeCO}_3 + \text{H}^+ \leftrightarrow \text{Fe}^{2+} + \text{HCO}_3^-$	Traps dissolved CO ₂ in mineral form

Table 10. Initial Aqueous Species Values in case of O₂ impurities simulation.

Species	Value (ppm)	Purpose/Role
pH	6.0	Slightly acidic baseline brine
Ca ²⁺	5000 ppm	Calcite dissolution/precipitation control
Mg ²⁺	2500 ppm	Dolomite reaction buffering
Na ⁺	90,000 ppm	Defines high-salinity brine, density effects
SO ₄ ^{2−}	1000 ppm	Links to anhydrite & sulfur reactions

Table 10. Cont.

Species	Value (ppm)	Purpose/Role
Fe ²⁺	36 ppm	Enables Fe redox cycle & siderite formation
Cl [−]	1000 ppm	Charge balance with Na ⁺

3.6.6. Output Parameters and Diagnostics

Time-series outputs (pressure, saturation, dissolved CO₂, mineral mass) and 3D property grids (porosity, permeability, molality) were extracted at identical milestones (end of injection, +10, +50, +100, +300, +500, 1000 years).

In addition, for each run, the following metrics were computed:

- Storage partitions: mobile, residually trapped, dissolved, and mineralized CO₂ masses
- Pressure evolution: reservoir pressure vs. time.
- Porosity and permeability reduction: spatial and temporal variation due to mineral precipitation.
- CO₂ molality: distribution in brine phase to indicate solubility fronts.

Furthermore, the following comparisons were made to analysis the CO₂ storage in different cases

- Physics mode comparison: evaluate incremental trapping and plume behavior across Modes 1–3.
- Rock type comparison: contrast clastic versus carbonate responses under identical conditions.

4. Results and Discussion

4.1. The Effect of Trapping Mechanisms

In an attempt to assess the individual contribution of the various trapping processes, three simulation runs were conducted. These four simulations were performed under the same operating conditions, which involved an injection period of one year and the total simulation time of 200 years. In Table 11, the four simulation runs, the various trapping processes were incrementally incorporated and compared.

Table 11. Effect of Trapping Mechanisms on CO₂ Distribution.

Case	Capillary (Residual) Trapping	Dissolution in Brine	Mineral Trapping	Mobile Supercritical CO ₂	Plume Spread & Migration
Base Case (No hysteresis/no mineral)	Very Low	Highest	None	None	Highest
+Hysteresis	Moderate	Reduced	None	None	Lower than base case
+Hysteresis + Mineral	High	Lower	Present (stable)	Moderate	Relatively Significant reduction
+Hysteresis + Mineral + Vapor	Strongest	Slight decrease	Highest	Minimal	Relatively most restricted plume

In case 1 (Structural + Solubility Trapping—Base Case), the trapping of CO₂ mainly occurs through structural trapping below the caprock and solubility trapping as CO₂ dissolves into the formation brine. In the injection phase and shortly after, most of the CO₂ cloud is expected to be mobile, and it would be dependent on the geometry of the reservoir and the integrity of the top seal for trapping. Subsequent solubility trapping

would increase the trapping as a result of the density difference created by the dissolution of CO₂.

Case 2 (Residual Trapping by Hysteresis) adds capillary trapping. Following injection cessation, the imbibition of the brine into the pore space Results in permanent trapping of the CO₂ ganglia that are disconnected. This rapid trapping process reduces the mobility of the plume, impedes upward migration, and increases the heterogeneity of saturations during the early injection period.

Case 3 (Mineral trapping and ion exchange) involves geochemical interactions between the dissolved CO₂ and the minerals present in the reservoir, trapping the CO₂ as precipitates of immobilized carbonates. Though it takes longer to develop, the trapping process provides the most secure method of CO₂ burial. Ion exchange adds an extra step for the irreversible immobilization of CO₂. At the close of the 200-year model run, the process provides considerably higher immobilization compared to the first two cases.

Case 4 (Vaporization + Mineral Trapping) considers all the above processes, as well as the vaporization of the formation water into the CO₂ phase. As the CO₂ interacts with the brine, the water vaporizes into the CO₂ phase, thus increasing the salinity of the brine and the geochemical reactions. These high salinity levels enhance the supersaturation of carbonates and their rapid precipitation around the CO₂ plume. On the other hand, the vaporization of water affects the permeability and the trapping capacity of the CO₂ by increasing the trapping efficacy as the water saturation levels decrease around the major CO₂ flow paths. This case illustrates the maximum improvement in the CO₂ trapping capacity, as it immobilizes the maximum amount of CO₂ and restricts the size of the detectable CO₂ plume. In general, the improvement from physical trapping alone (Case 1) to complete immobilization involving trapping by capillary, geochemical, and vaporization mechanisms (Case 4) illustrates an increase in the degree of storage and pressure, and trapping capacity. These results show the benefit of incorporating trapping mechanisms involving petrophysics and geochemical processes during the development and evaluation of the site for carbon capture and storage.

Figure 4 indicates the average reservoir datum pressure for the four different CO₂ storage scenarios: the base case, hysteresis, hysteresis with mineral reaction processes, and hysteresis with both mineral reaction processes and vaporization. For all cases, during the injection period the pressures show a rapid increase representing the injection of the CO₂ and then follow a stable path once the injection ceases.

In the base case, the stabilized pressure is the lowest. This is due to the absence of other trapping mechanisms that allow more CO₂ to be in the supercritical fluid phase, which is able to distribute more efficiently in the reservoir, thereby resulting in lower stabilized pressures.

Inclusion of hysteresis results in a slightly higher average pressure compared to the base case. Residual trapping causes a certain portion of CO₂ to get stuck in the pore space, resulting in reduced permeability and mobility. Consequently, dissipation of pressure becomes less effective, thereby increasing the average pressure.

The maximum values of pressure occur in those scenarios that involve mineral reactions, both with and without vaporization. Mineral entrapment causes a reduction in dissolved CO₂ content to form solid carbonate minerals, which in turn leads to a decrease in the pore volume, thereby causing high values of pressure in comparison to scenarios involving physical entrapment.

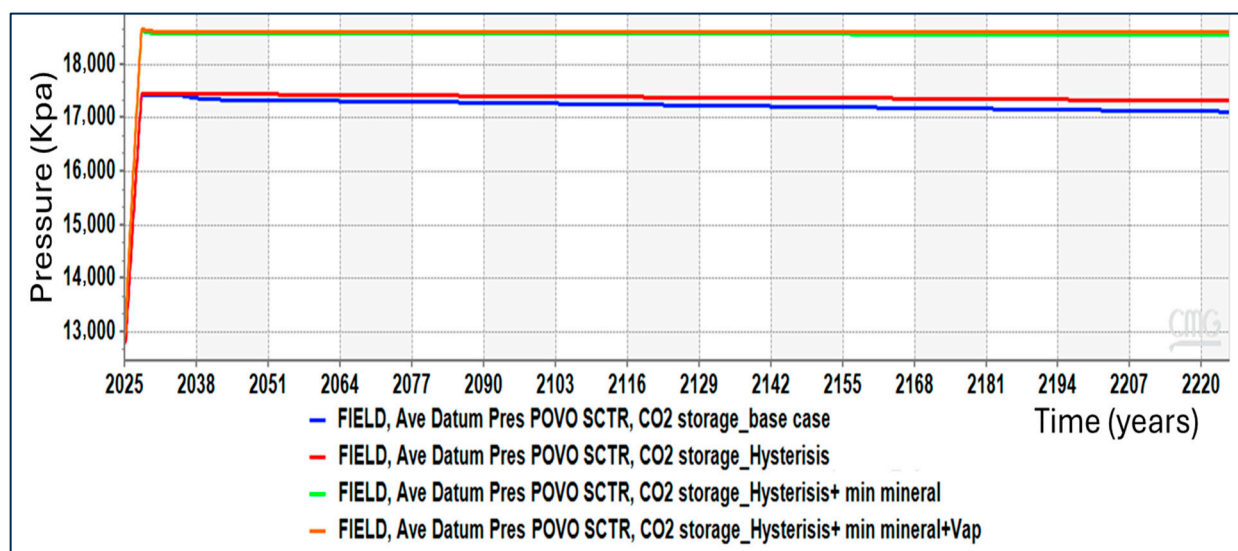


Figure 4. Average Pressure vs. Time.

In addition, the introduction of vaporization has no marked impact on the overall trend of system pressure compared with that of the mineral system only scenario, which further implies that the contribution of vaporization is limited to the local fluid distribution around the well rather than influencing overall system pressure. On the other hand, the calculation results show that geochemical trapping enhances storage security yet simultaneously causes elevated storage system pressures.

Figure 5 compares the evolution of supercritical CO₂ (free-phase CO₂) for four modeling cases: the base case, hysteresis only, hysteresis with mineral reactions, and hysteresis with mineral reactions and vaporization.

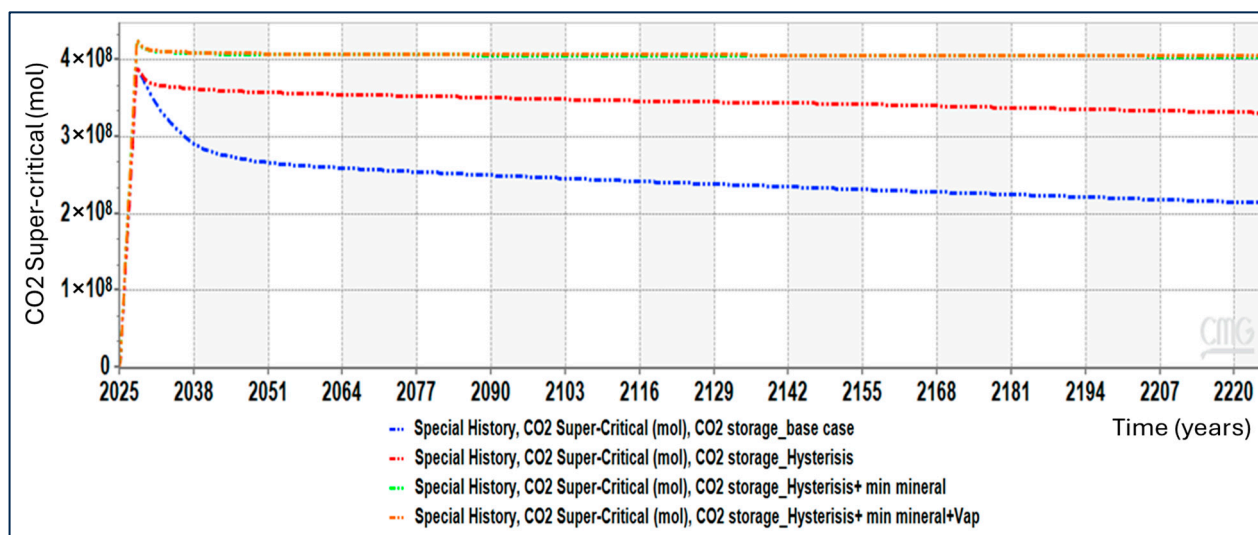


Figure 5. CO₂ supercritical vs. Time.

In the base case, supercritical CO₂ shows the largest decline with time. Because no trapping mechanisms are activated, CO₂ remains fully mobile after injection. Following injection shut-in, the supercritical CO₂ plume continues to redistribute and migrate due to buoyancy and pressure dissipation. The observed reduction in supercritical CO₂ therefore reflects plume spreading and loss of structural containment, not immobilization.

When hysteresis is enabled, the decline in supercritical CO₂ is noticeably reduced. Residual trapping occurs during post-injection imbibition, converting part of the mobile

CO₂ into immobile residual gas. This limits further migration and stabilizes the supercritical CO₂ volume compared to the base case.

The inclusion of mineral reactions further stabilizes the system. Although mineral trapping is a slow process, it gradually consumes dissolved CO₂, indirectly reducing the amount of CO₂ available to remain in the free supercritical phase. As a result, the supercritical CO₂ curve becomes flatter over time, indicating enhanced long-term containment.

Finally, when vaporization is included, the supercritical CO₂ remains the most stable and highest among all cases. Phase partitioning between aqueous and gas phases reduces effective CO₂ mobility and limits free-phase redistribution. This combination produces the strongest immobilization behavior, even though injectivity may be reduced elsewhere in the system.

Figure 6 indicates that the CO₂ dissolved history is strongly dependent on the trapping mechanisms that are activated, thus illustrating the interaction between solubility trapping and residual, mineral, as well as phase effects. In the base case simulation, where only structural trapping is operational, the amount of CO₂ dissolved is at its highest level and continues to rise steadily with each annual simulation step. This is because a large amount of the injected CO₂ remains in the supercritical phase with high mobility, allowing considerable interaction between the phase and the brine in the formation.

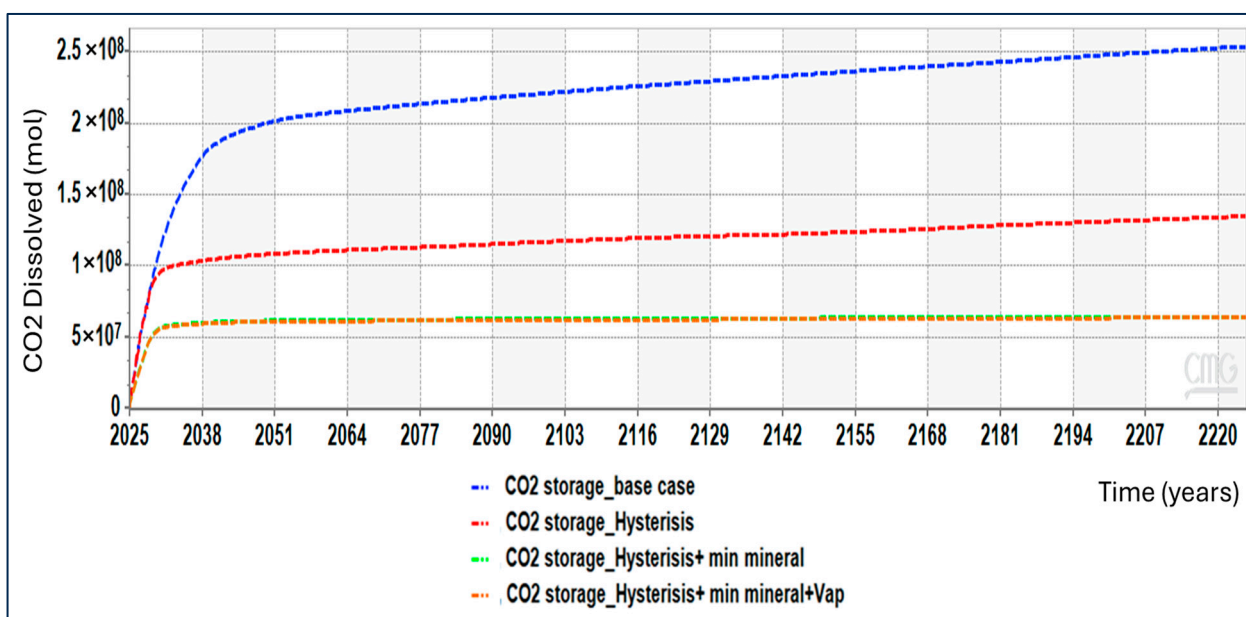


Figure 6. CO₂ Dissolved vs. Time.

When hysteresis is considered, the amount of dissolved CO₂ is decreased compared to the reference case. Hysteresis favors the entrapment of the gas by forming disconnected ganglia that get immobilized during the drainage and imbibition processes. This reduces the amount of supercritical CO₂ that is in contact with the aqueous phase. Although solubility trapping occurs in this case, the rate at which the dissolved amount increases and the amount at the end are much lower compared to the previous case.

The addition of mineral reactions results in a further decrease in the amount of dissolved CO₂. In this scenario, the CO₂ which diffuses into the brine will also react chemically to form solid carbonate minerals. This process, which moves CO₂ from the aqueous phase to the mineral phase, competes directly with solubility trapping. Consequently, the concentration of dissolved CO₂ tends toward a much lower equilibrium, which signifies the role of mineral trapping as a long-term sink for the build-up of dissolved CO₂.

When the effects of vaporization are included on top of hysteresis and mineralization, the dissolved CO_2 concentration is found to be the lowest among all cases. Vaporization changes the phase equilibrium and decreases the solubility of CO_2 in the aqueous phase, and mineral reactions continue to consume dissolved species. The effect of all these processes is to limit the evolution of dissolved CO_2 concentrations substantially after injection and cause the dissolved CO_2 concentration to stabilize at a considerably early stage. This is because CO_2 is being preferentially transferred to trapped and mineralized fractions. In summary, the graph indicates that the increased level of CO_2 in solution is not necessarily related to strong storage security. Indeed, although the CO_2 solution level is the highest in the basic scenario because solubility trapping is continually occurring, the basic scenario has no trap mechanisms for residual and mineral storage. Conversely, storage scenarios where hysteresis, mineralization, and vaporization occur display lower levels of CO_2 in solution but improved storage security because multiple trapping mechanisms are at play.

In Figure 7, it is evident that the distribution areas of CO_2 molality vary significantly between the four scenarios due to the increasing activation of secondary trapping processes. In the base case, where structural and solubility trapping alone are simulated, the dispersed zone of dissolved CO_2 is largest and most extensive, signifying high mobility and frequent interaction between the CO_2 phase and formation brine. As hysteresis (residual trapping) is incorporated into the processes, the areas with high dissolved CO_2 become restricted, signifying immobilization of injected CO_2 amounts earlier, which are, in turn, beyond the dissolution influence of fresh brine. Incorporation of mineral trapping decreases the areas and magnitudes of dissolved CO_2 , signifying utilization of CO_2 amounts during geochemical reactions, forming solid carbonate minerals. The last option, involving vaporization + mineral trapping, has the lowest areas and magnitudes of dissolved CO_2 . Water vaporization decreases the formation brine saturation and formation brine salinity, which are factors hindering the dissolution of CO_2 .

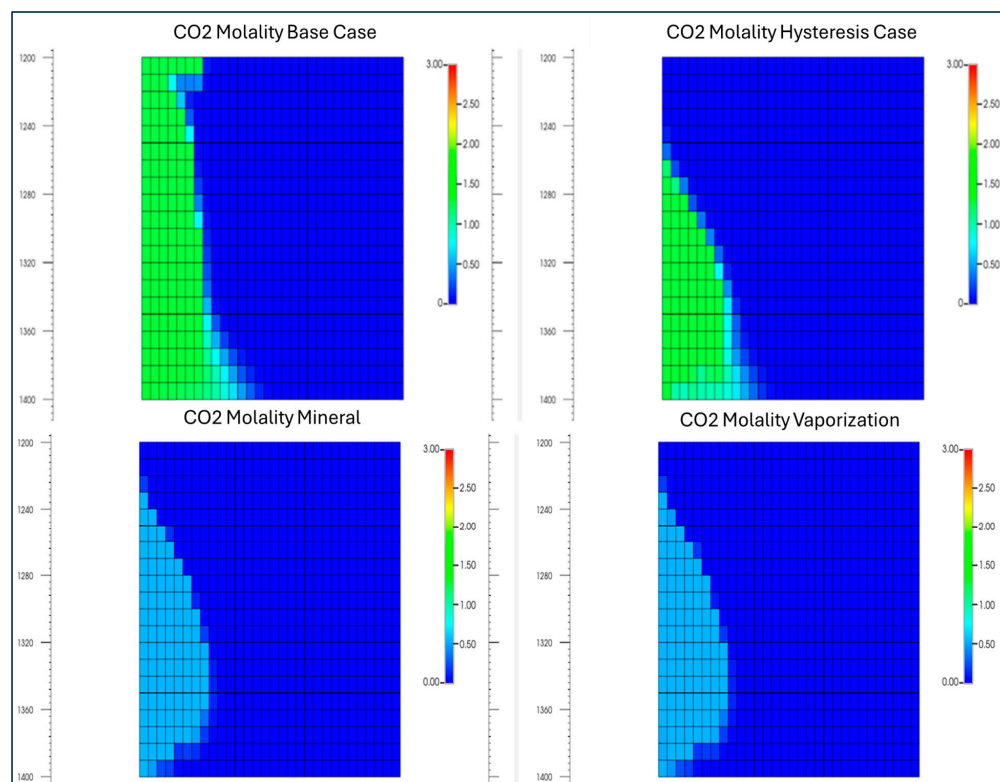


Figure 7. Comparison of CO_2 Molality in the Four Cases.

Thus, these findings corroborate the fact that with the ever-increasing number of trapping mechanisms activated (from hysteresis to mineralization to vaporization), the dissolution phase of CO₂ is constantly restricted and localized, which increases the overall containment security and further decreases the active dissolution plume extent within the reservoir.

Figure 8 displays a comparison between the capillary-trapped CO₂ saturation (Sgr) maps after 200 years, including four trapping geometries. Residual trapping behavior is very much dependent on the immobilization processes occurring during and after the CO₂ injection.

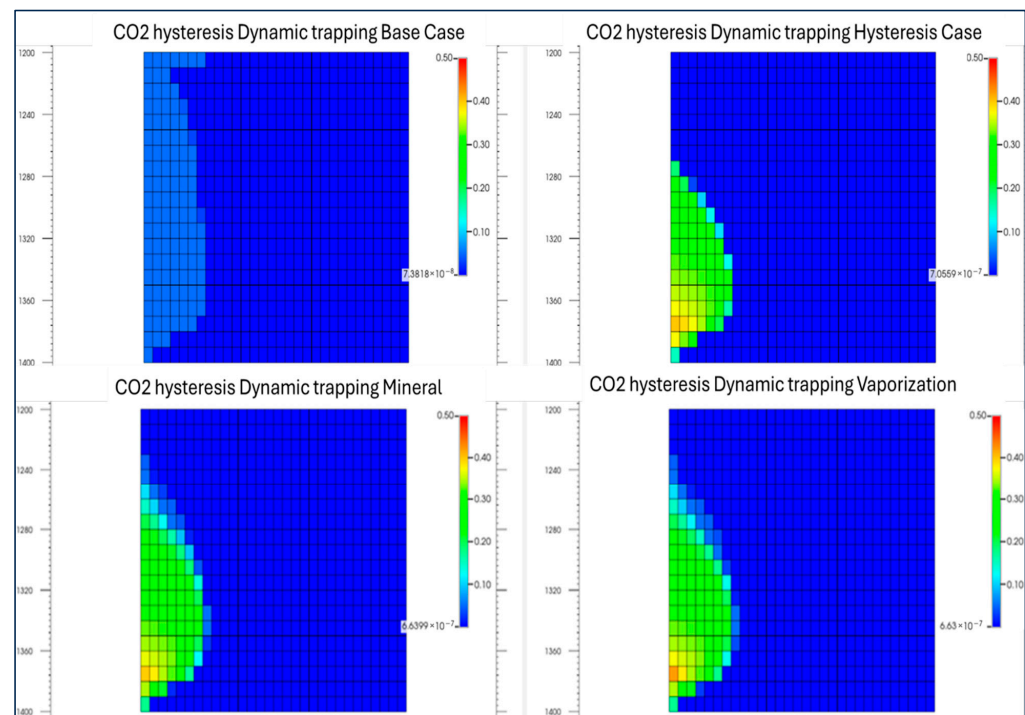


Figure 8. Residual CO₂ Saturation (dynamic trapping) differences in the Four Cases.

In the base case, the hysteresis is off, and consequently, most of the injected CO₂ is mobile. The CO₂ plume is buoyant and accumulates structurally without much permanent trapping. Consequently, the reservoir has zero Sgr, which suggests a high potential for long-range migration if not trapped by structure.

When hysteresis is considered, capillary trapping becomes active after injection is completed and brine starts to imbibe back into the rock. The CO₂ zone moves very quickly and is trapped as individual ganglia. This creates a sharp, crescent-shaped zone of residual CO₂ surrounding the injection zone, which accurately reflects fluid invasion and displacement. In this example, it is evident that the very strong trapping effect is associated with the first line of immobilization following shut-in.

With the addition of mineralization, the result is a more focused and smaller trapped plume. The mechanism of mineralization adds carbonates to the system by reacting part of the dissolved CO₂ into more stable carbonates, particularly near the injection point. As more mobile and dissolved CO₂ is consumed by reaction, the amount of CO₂ left to migrate and develop new locked clusters decreases. Decisions based on the volume changes of Sgr are a straightforward measure of increased long-lasting trapping.

Lastly, the extent of the most compact plume is attained by the vaporization + mineral trapping mechanism. The result of water vaporization into the simulated CO₂ flow is to reduce brine saturation and increase salinity. This regime is interpreted to moderately

influence capillary pressure and modification of the respective permeability, delaying the start of residual trapping but impeding the expansion of the plume. Although the difference is slight, the front is not merely more contracted, but also fixed, and has little possibility of buoyancy-assisted movement.

In Figure 9, the pH distribution after 200 years is shown for the four trapping processes, illustrating brine acidity changes with increased immobilization processes. In the base case, the pH value is constant and basic over the entire domain because very little CO_2 is soluble within the formation water. As a result of the supercritical mass of CO_2 being trapped structurally, and when little carbonic acid is generated, the geochemistry of the formation brine is not significantly affected. In the hysteresis-only case, the inclusion of residual trapping is also ineffectual, and as most of the CO_2 is isolated in unconnected pockets, little interaction takes place, and consequently, the geochemistry is unaffected.

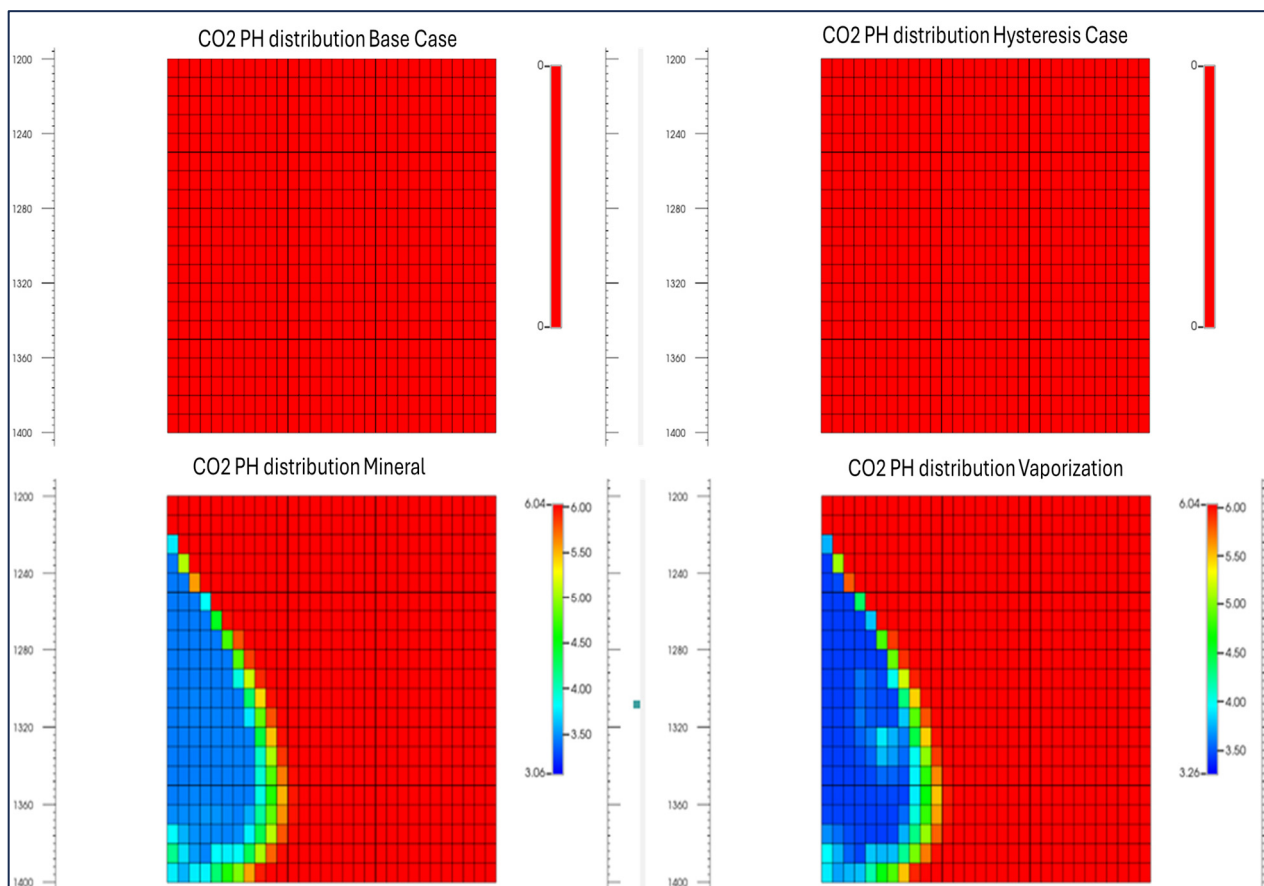


Figure 9. Comparison of pH Distribution Across the Four Trapping Cases.

A significant transition is realized when mineral trapping is enabled. In the case of hysteresis + mineralization, a strong low-pH area is realized around the CO_2 blob, signifying active dissolution of CO_2 . When CO_2 is dissolved, it combines with water to form carbonic acid, which is a strong sign of carbonates forming. The sour areas are also known to show where geochemical transformations are attained, which translates to converting dissolved CO_2 into a more stable form. As of 2225, the areas are still sour, signifying a high level of geochemical trapping.

The hysteresis, mineralization, and vaporization process further exacerbates such phenomena. The vaporization of water into the CO_2 phase causes dehydration and increased saturated brine and salinity within the surrounding areas of the injection site, which favors the dissolution and reaction rate of CO_2 . Consequently, a greater and more active zone of

acidity is produced compared to the case involving mineralization. This suggests not only increased dissolution of CO₂ but also an intensified geochemical reaction process. Overall, it is evident from the comparison that the extent of geochemical interaction between CO₂ and rock is very important to control the changes of pH. When only the physical trapping mechanism is used, there are negligible chemical changes. With the inclusion of mineral reactions, it initiates the long-term process of stabilization. When further consideration is given to the effects of vaporization, dissolution and conversion processes are further increased, which also increases the ability to buffer. Therefore, it can be said that the changes in pH are very significant to assess the efficiency of chemical trapping.

Noticeable change happens when mineral trapping becomes a factor. Looking at the hysteresis + mineral scenario, the strong Acidic Halo develops around the CO₂ patch. This indicates the locations where the dissolved CO₂ reacts with the water to form carbonic acid.

The regions demonstrate the onset of the irreversible storage process of the CO₂, where the gas migrates from being a fluid to a solid mineral form. This clearly demonstrates how mineral trapping factors directly improve storage efficiency by reducing the overall amount of free CO₂ in the simulation.

The greatest degree of geochemical influence takes place when the degree of vaporization is estimated. The highest degree of the hysteresis + mineral + vaporization effect demonstrates the largest degree of acidification. Water vaporization to form CO₂ effects high salinity of the brine and decreases the saturation of the aqueous systems. The dissolution of the CO₂ accelerates mineral reactions. This contributes to a larger chemically altered region together with a faster transition to a steady-state mineral form. The pH effect demonstrates the degree to which the vaporization influence accelerates the immobilization of the chemical processes. Taken together, these findings demonstrate that pH sensitivity serves as a highly informative factor for the efficiency of geochemical trapping in CO₂ storage. In the case of scenarios without mineral reactions, there is very little variation in pH values, demonstrating the ineffectiveness of physical trapping in converting CO₂ into a less harmful form over a long period of time. When chemical processes become operational, the acidity in the reservoir develops in a manner proportional to dissolution rates and the range of mineralization. The expanded region of acidity in the scenario of vaporization enhancement further substantiates the optimistic effects of combining different mechanisms of trapping in terms of both magnitude and rapidity for permanently storing CO₂.

4.2. The Effect of Simulation Time

The long-term transition of the CO₂ for the scenario including all the mechanisms of storage (structural storage, hysteresis/residual storage, dissolution storage, mineral storage) and the effect of the vaporization of the water for the transition of the CO₂ from the supercritical to the mineralized phases. A total of 10 years of injection was assumed in the scenario for the total simulation time of 1000 years.

At the initial stages of the injection process, a gross amount of CO₂ stays in the supercritical phase to occupy the entire possible pore space around the wellbore. After ceasing the CO₂ injection processes, the amounts of the supercritical CO₂ slowly begin to reduce. Figure 10 represents a clear indication of the gradual immobilization of gas. Additionally, the supercritical gas phases take a decade or two to become stable.

Residual trapping begins to rise more sharply at the end of the injection phase, where the smaller ganglia of CO₂ remains trapped in the rock pore space. Dynamic residual immobilization takes place at the end of the modeling period in the earlier centuries, where the trapped CO₂ slowly mixes into the brine.

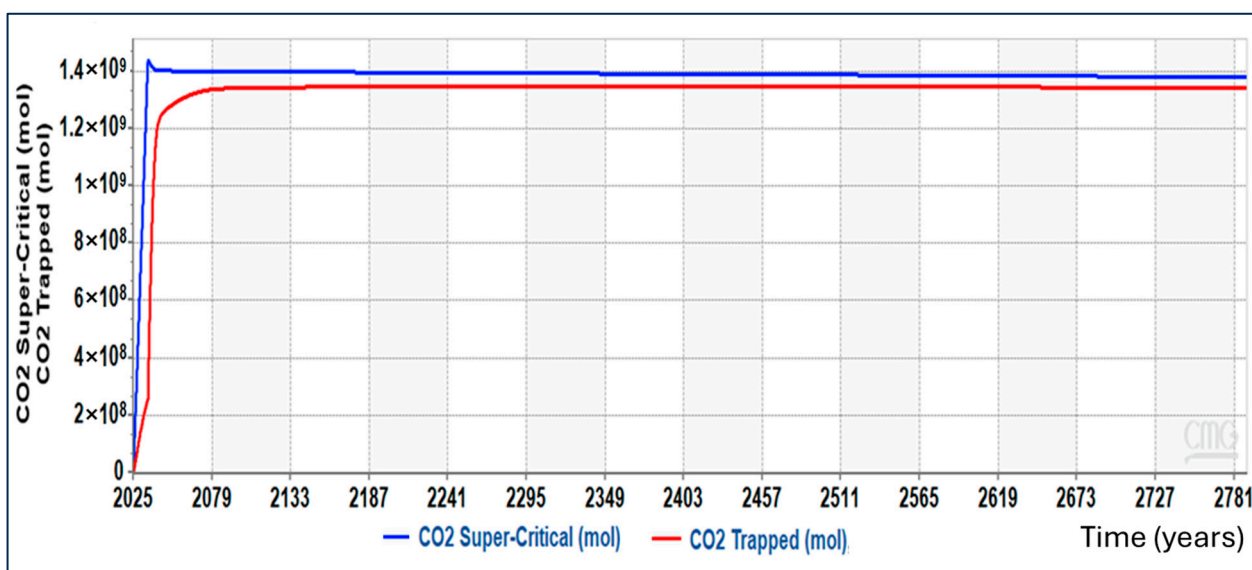


Figure 10. Comparison of CO₂ supercritical vs. trapped in the long-term (1000 yrs).

Figure 11 shows that the amount of dissolved CO₂ continues to grow significantly in the simulation as the concentrations of the supercritical and residual phases decrease. This occurs due to the interface made in the plume migration. Dissolution plays a vital role in the simulation since the CO₂ becomes less buoyant. Additionally, the CO₂ migrates in the form of dense brine instead of being trapped in the bottom of the cap rock. The steady dissolution of CO₂ in the simulation makes the process of solubility continue to trap CO₂ over a long period of centuries.

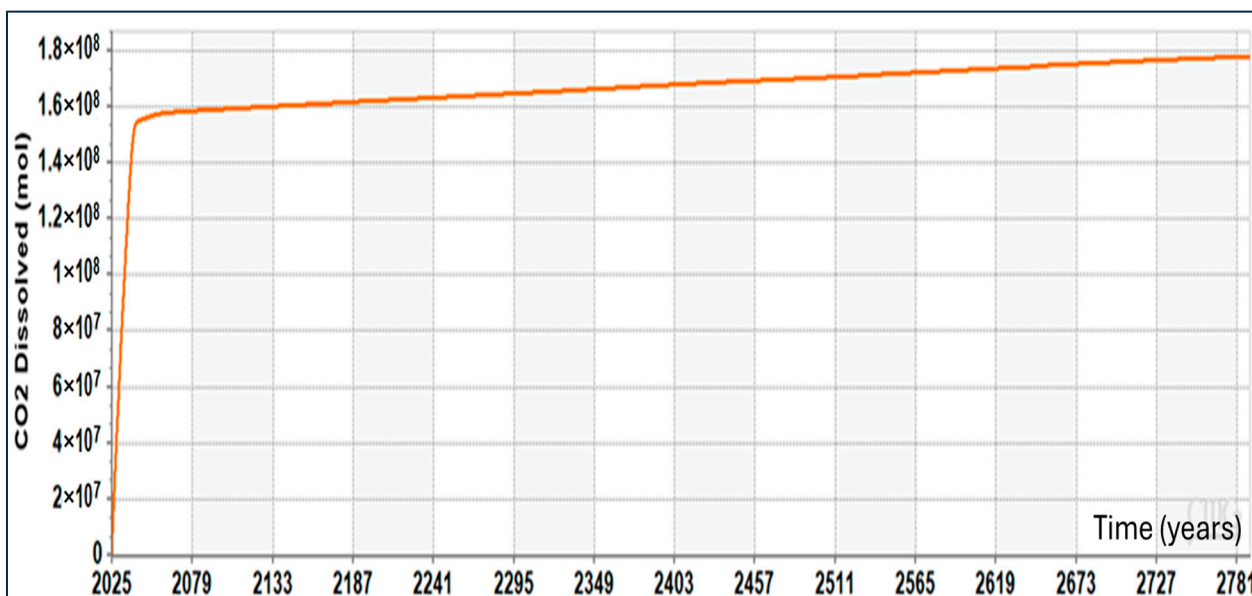


Figure 11. CO₂ Dissolved trend over decades.

Mineral trapping like in Figure 12 has a slower growth process but involves the strongest guarantees of immobilization. With the reaction of dissolved CO₂ concentrations in the formation brine and mineral substances, there is a gradual build-up of carbonate. A strong growth in mineral trapping in the initial years following the end of injection represents highly reactive geochemical environments in the vicinity of the plume. After the initial years (till the end of the first hundred years) of higher mineralization rates

corresponding to the depletion of reactive mineral substances, there would be a gradual fall in mineralization.

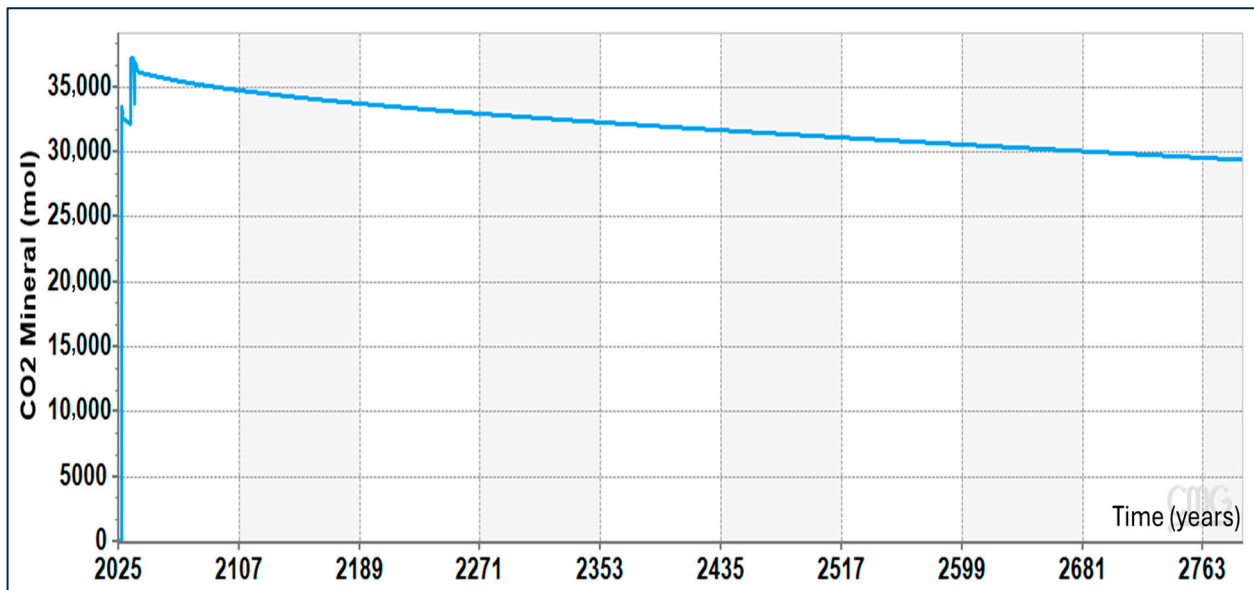


Figure 12. CO₂ mineralization trend over decades.

Aqueous ion tracking in Figure 13 validates the chemical process as the level of dissolved inorganic carbon remains high, supporting the contention of continuous mineralization but under the control of reaction rates. In the latter stages of simulation, the system tends toward a steady state between the dissolved and mineralized phases, signifying a gradual shift from a short-term physical trap to a long-term trap.

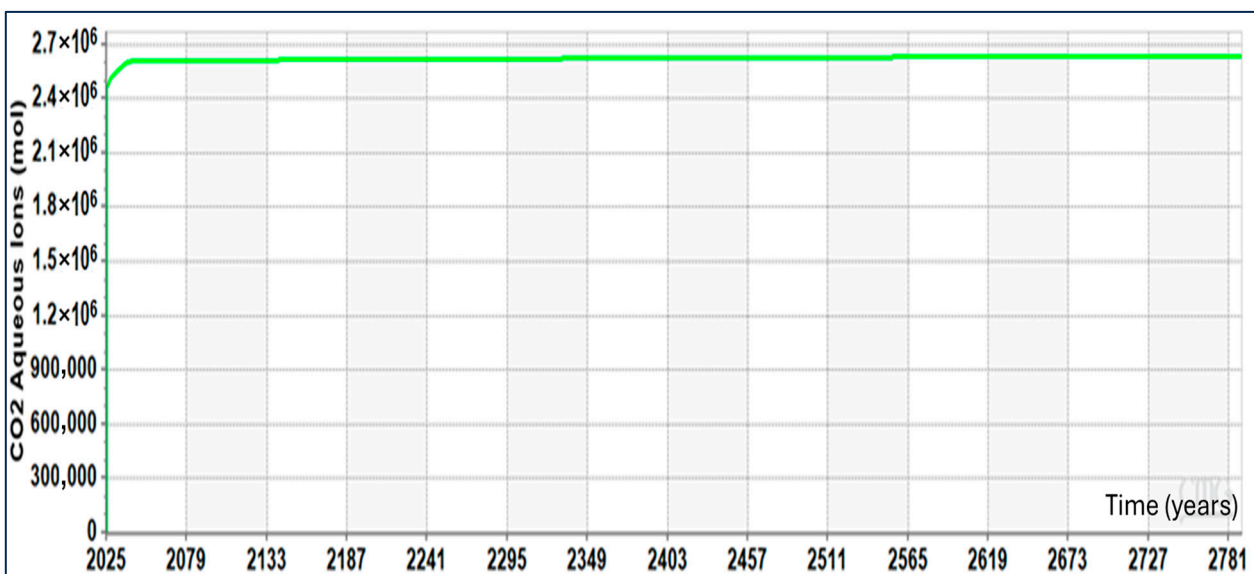


Figure 13. CO₂ Aqueous ions trend over decades.

Taken together, these findings indicate that the supremacy of the supercritical/residual phase reduces over the years until dissolution/mineralization becomes the prevailing processes. At the 1000-year point, most of the trapped gas is in the dissolved/mineral phases, thereby greatly improving the safety of gas storage. These findings support the efficiency of the combination of the different gas storage mechanisms. Hysteresis provides early gelation for improved gas safety in the short term. Solubility/minerals offer long-term

storage. Comparison between the different simulation times scenarios is listed below in Table 12.

Table 12. Comparison between simulation time scenarios.

Parameter	200 yrs	500 yrs	1000 yrs	Trend with Time
Free supercritical CO ₂	decline	Major decline	Nearly zero	Strong stability gain
Capillary trapped CO ₂	High	Stable	Stable	Immobilization complete early
Dissolved CO ₂	Slightly Increased	Increased	More Increased	Ongoing reactive trapping
Mineral CO ₂	Low	Moderate	High	Main long-term trapping

4.3. The Effect of Different Rock Types, Salinity and O₂ Impurities

Given the importance of the mineral composition of the reservoir rock and the aquifer to the efficiency of dissolution, ion exchange, and mineral trapping, a sensitivity test has also been conducted to assess the role of rock types towards CO₂ long-term containment. In consideration of further geochemical reactions triggered by oxygen impurities within the injected CO₂ stream, which has the ability to expedite mineral dissolution and further influence brine chemistry and carbonate precipitation, research has also assessed the role of oxygen impurities.

4.3.1. Clastics vs. Carbonates

Figure 14 presents a comparison of the pH distribution after 200 years for the two sets of rocks reactivity assumptions. In both cases, there exists a clear region of acidity in the vicinity of the CO₂ plume due to the dissolution of CO₂ into the brine, thereby forming the initial steps of the carbonic acid. There seems to be a variation in the magnitude of the acidity in terms of spatial distribution. In Figure 14 the Clastics (sandstone) scenario, the region of dissolution seems to be less in width compared to the carbonates scenario. This suggests the rates of geochemical processes to be slower in the traditional carbonate scenario. This indicates a lower degree of action between the fluid phases in the Clastics scenario.

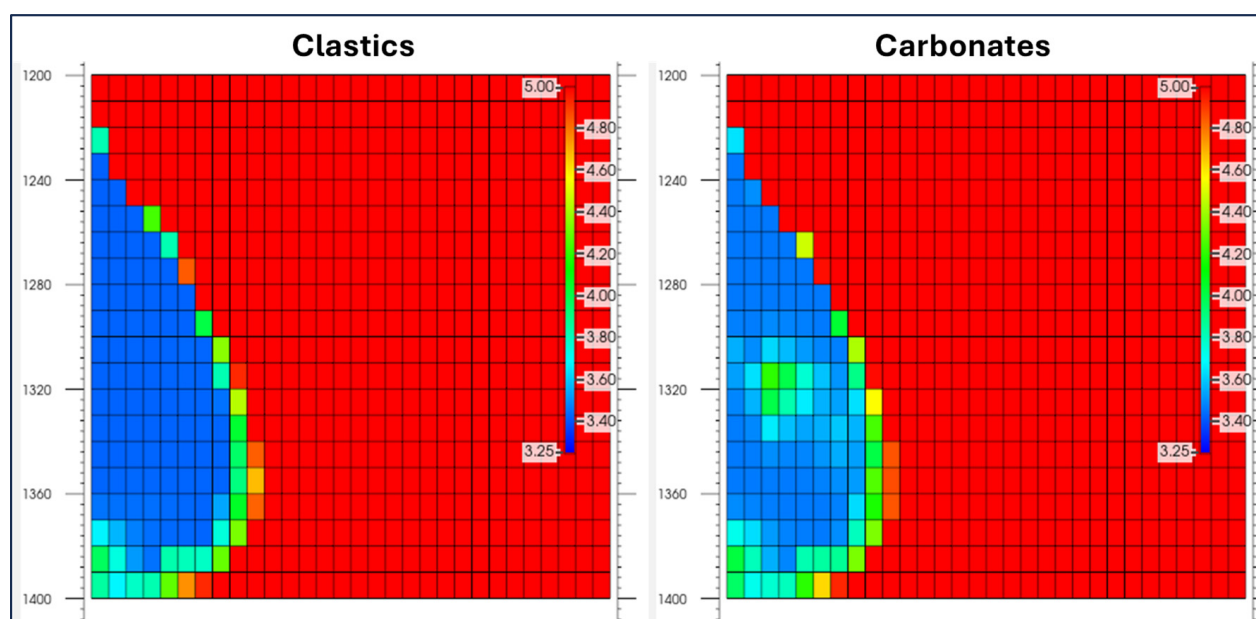


Figure 14. Clastics vs. Carbonates pH distribution.

In contrast to the previous case, when the concentrations of the carbonate mineral phases of higher reactivity become higher, the area of the low pH region significantly

expands. An extended acidic region points to a higher dissolution speed as the carbonate mineral phases actively take parts in the neutralization of dissolved CO₂ in the region. At the same time, the region promotes the dissolution of CO₂ into carbonate mineral phases. A higher degree of dissolution in the carbonate mineral phases indicates the improved capability of the trap to confine CO₂ in the long term since a higher degree of dissolution of CO₂ takes place in the trap.

Taken together, these findings make it clear that the carbonate mineral composition of the rock plays a pivotal role in the long-term storage of the CO₂ as stated in Table 13. A rock that has high reactive carbonate not only helps in the rapid neutralization of the acid but also allows more rock to be a contributing factor in mineral entrapment. Vaporization makes this even more efficient by allowing the brine to have a higher salinity level. This would allow more CO₂ to undergo a chemical change to become a more stable form over a long period of time.

Table 13. The combined effect of salinity concentration and rock type.

Salinity Concentration	CO ₂ Dissolved (Molality)	pH Drop	Precipitated Carbonate	Plume Lateral Spread	Overall Storage Security
5000 ppm	Medium	High acidity region	Low	Moderate	Moderate
50,000 ppm	Higher	Better buffering	Higher	Slight change	Good
200,000 ppm	Highest	Best buffering	Maximum	Slightly smaller	Excellent

4.3.2. Effect of Salinity

Figure 15 demonstrates the molality distribution of CO₂ in carbonate formations with varying values of calcite availability: Ca = 5000; 50,000; and 200,000. In the minimum carbonate scenario (Ca = 5000), the molal concentration of dissolved CO₂ is highest around the edge of the CO₂ plume. The molal gradient in the figure is very sharp and localized. The effect of a small contact area between the supercritical fluid plume and the aqueous phase suggests that dissolution-controlled trapping mechanisms may be less favored.

With the enhancement of the calcite concentration to Ca = 50,000, the region of high CO₂ molality definitely extends to a larger area around the edge of the plume. This enhancement of molality demonstrates a higher dissolution of CO₂. This is particularly linked to the high rates of reaction/mixing pathways supported by high mineral concentrations. With high concentrations of carbonate surface regions being more susceptible to dissolution, the interface between the plume and the brine will extend, thereby enabling a higher dissolution of the CO₂ from the mobile gas phase to the chemically dissolved phase.

The high carbonate case (Ca = 200,000) exhibits the strongest dissolution characteristics. In the high carbonate case simulation, the molality plume extends further into the reservoir. The larger dissolution interface in the high carbonate case simulation also indicates the enhancement of the geochemical effect. More reactive interfaces continue to be produced due to the dissolution of carbonate material. Such dissolution further enhances the solubility of CO₂ gas. Consequently, the storage safety increases since more of the stored CO₂ gas moves to the less mobile aqueous phase.

Taken together, these findings indicate that the presence of carbonate-rich formations significantly enhances solubility trapping capabilities. The higher reactivity of the mineral content would lead to a larger contact surface between the CO₂ molecules and the brine. Additionally, the dissolution rates would be higher. These characteristics would allow the dissolved CO₂ to extend beyond the immediate well location. Indeed, the dissolution of the CO₂ into the brine makes it denser. At the same time, there would be no risk of

buoyancy-related leakage. This would be accompanied by the conversion of CO_2 into solid carbonate minerals.

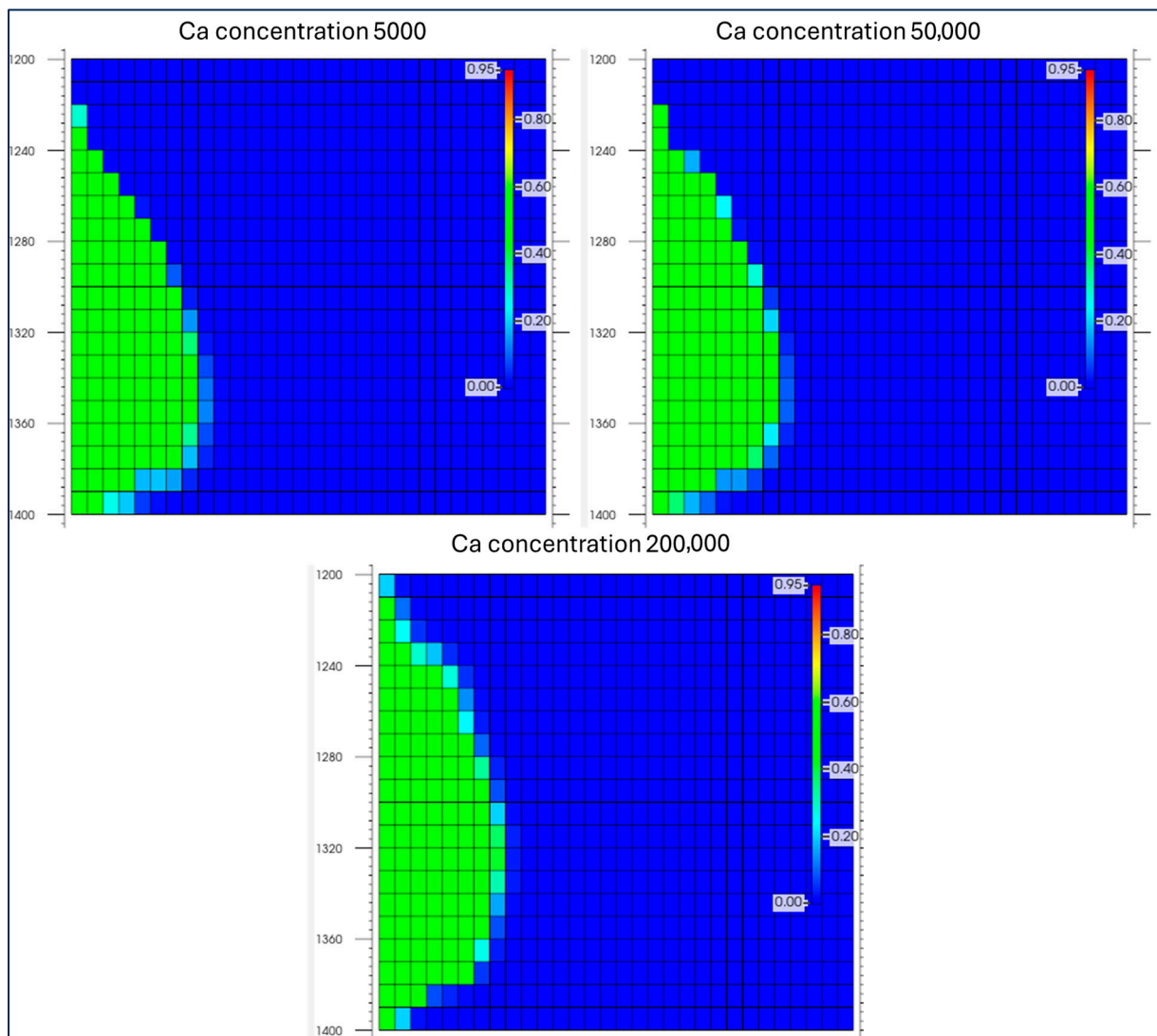


Figure 15. Effect of calcites (calcium in this case) concentration on CO_2 Molality.

Figure 16 presents the residual CO_2 saturation distribution after 200 years for carbonate reservoirs with increasing calcite abundance ($\text{Ca} = 5000$; $50,000$; and $200,000$). In every case, residual trapping occurs primarily along the trailing edge of the CO_2 plume, where gas has displaced brine, migrated outward, and subsequently become immobilized as pore-scale ganglia. However, the magnitude and areal extent of this trapped zone evolve significantly as a function of carbonate mineral availability. In the low-carbonate case ($\text{Ca} = 5000$), the plume footprint is relatively narrow and only the immediate zones swept by the plume show meaningful residual gas saturation. Because the formation has limited reactivity, dissolution is weak and only a small amount of CO_2 transfers into the brine. As a result, the supercritical plume retains a more compact geometry, and snap-off trapping is constrained to a limited volume.

When carbonate availability increases to $\text{Ca} = 50,000$, the spatial coverage of trapped CO_2 increases and the saturation gradients become more smoothly distributed. This is attributed to enhanced dissolution and fluid rearrangement along the plume boundary. As CO_2 dissolves and weakens buoyant drive, plume migration slows and lateral expansion increases, creating broader regions of capillary snap-off and disconnection from the mobile

phase. Thus, the enhanced geochemical reactivity indirectly amplifies residual trapping by encouraging more uniform plume thinning and more sustained contact with brine-filled pore structures.

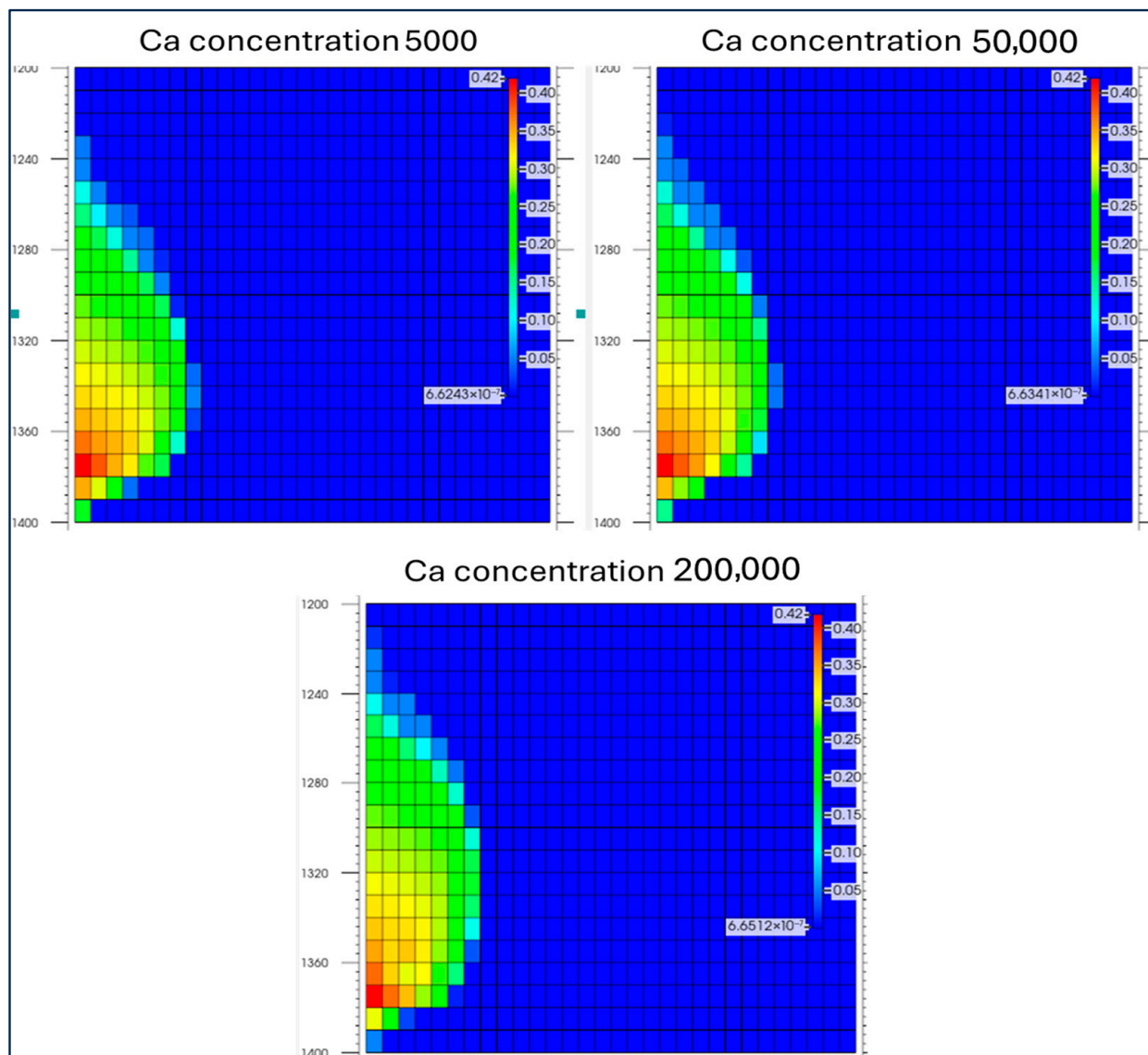


Figure 16. Effect of calcites (calcium in this case) concentration on CO₂ Residual rapping.

The strongest trapping response is observed in the most carbonate-rich case (Ca = 200,000), where the residual CO₂ footprint expands dramatically and the saturation contours reach deeper into the reservoir. With a highly reactive matrix, continuous dissolution along the plume flanks increases brine–CO₂ contact efficiency and prolongs gas–liquid interface exposure. This drives extensive disconnection of CO₂ threads into isolated clusters, significantly boosting the volume of residually immobilized gas. Moreover, the broad spread of trapped gas indicates that dissolution–mineralization reactions are actively reshaping flow pathways, reducing vertical buoyant rise and encouraging lateral trapping instead of plume coalescence under the caprock.

Importantly, this behavior demonstrates that residual trapping is not purely physical in carbonate reservoirs—it is strongly coupled to geochemical processes. Greater carbonate availability leads to more dissolution, weakening the supercritical plume and promoting immobilization. At the same time, increased dissolution exposes new mineral

surfaces, reinforcing a feedback loop where CO₂ progressively transitions into less mobile states. Therefore, as mineral abundance increases, residual trapping evolves from being a short-term containment mechanism to becoming a major contributor to long-term plume stabilization. This synergy between capillary forces and dissolution means that carbonate-rich reservoirs provide more robust early and intermediate trapping security, even before mineral precipitation dominates.

Ultimately, these results show that carbonate formations do not just enhance chemical storage; they also substantially strengthen the physical immobilization of CO₂ through dynamic plume redistribution and improved contact efficiency. This dual trapping reinforcement underscores why carbonate reservoirs are among the most effective geological formations for CCS, offering secure, multi-mechanism immobilization that continues to improve with time.

Figure 17 demonstrates the progression of the extent of the brine phase change due to the injection of CO₂ in carbonate formations having different amounts of calcite. In the scenario having the lowest Ca concentration (Ca = 5000 ppm), the extent of the chemical change in the acidic phase can be considered to be more localized. There may be more dense regions of low pH values close to the boundaries of the plume. This may be due to the nature of the rock being less buffered.

There would be the formation of a sufficient amount of carbonic acid due to the dissolution of the higher amounts of dissolved CO₂. But the rock would have less capability to react.

With the higher carbonate concentrations reflected by the corresponding Ca = 50,000 values, the low-pH region extends both horizontally and in-depth. An enlargement of the region suggests more aggressive interactions between CO₂, the brine phase, and the rock mass. More calcite interfaces translate to favored dissolution reactions for the carbonate rock. Such chemical reactions result in a higher consumption of the formed carbonic acid. Hence, the corresponding regions representing the acidification process appear more distributed.

The largest degree of acidification takes place in the high-calcite case (Ca = 200,000). In this simulation case, there exists a very large amount of the plume interface region in the highly lowered regions of pH values. Such a degree of reactive carbonate chemistry clearly points to a very reactive carbonate system in which a reactive surface of the mineral undergoes continuous dissolution. At the same time, the reacted carbonate mineral surface keeps enough path length ahead to allow migration of the carbonic acid before being consumed. Additionally, the widened halo of the degree of acidification clearly indicates that a larger portion of the reservoir undergoes the action of the immobilization. Table 13 summarizes these findings demonstrate a positive and definite influence of carbonate mineral content on the strength of geochemical entrapment.

With higher Ca concentrations, there would be a greater dissolution interface for the dissolved CO₂ to react with the rock minerals, thus hastening the conversion of mobile CO₂ into solid form. Such a continuous buffering action would therefore promote the permanence of storage. The existence of carbonate mineral environments would therefore have outstanding benefits in the storage of CO₂ in the sense that storage would not only occur efficiently but also in a manner that emphatically guarantees storage permanence.

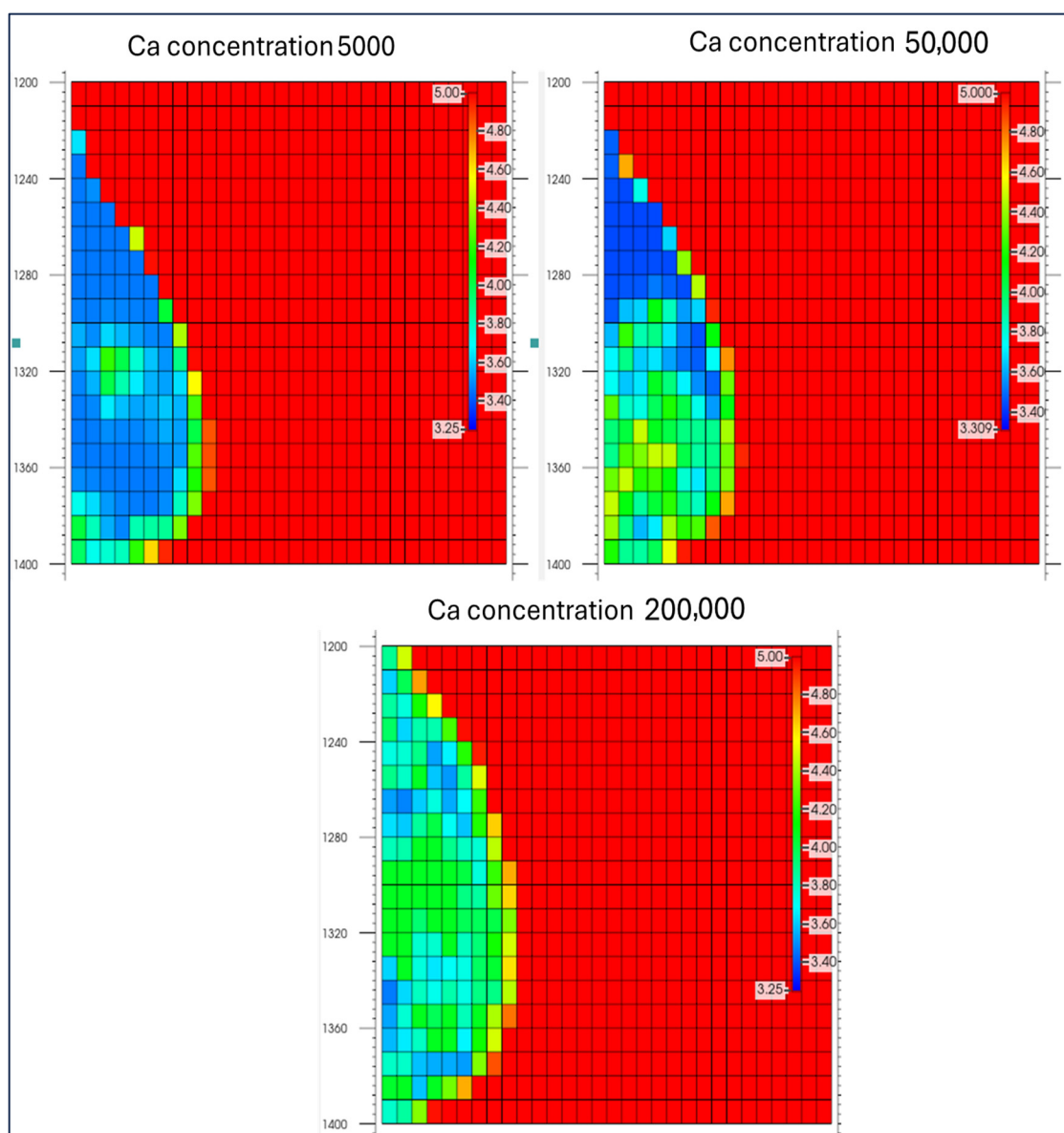


Figure 17. Effect of calcites (calcium in this case) concentration on pH distribution.

4.3.3. Effect of O₂ Impurity

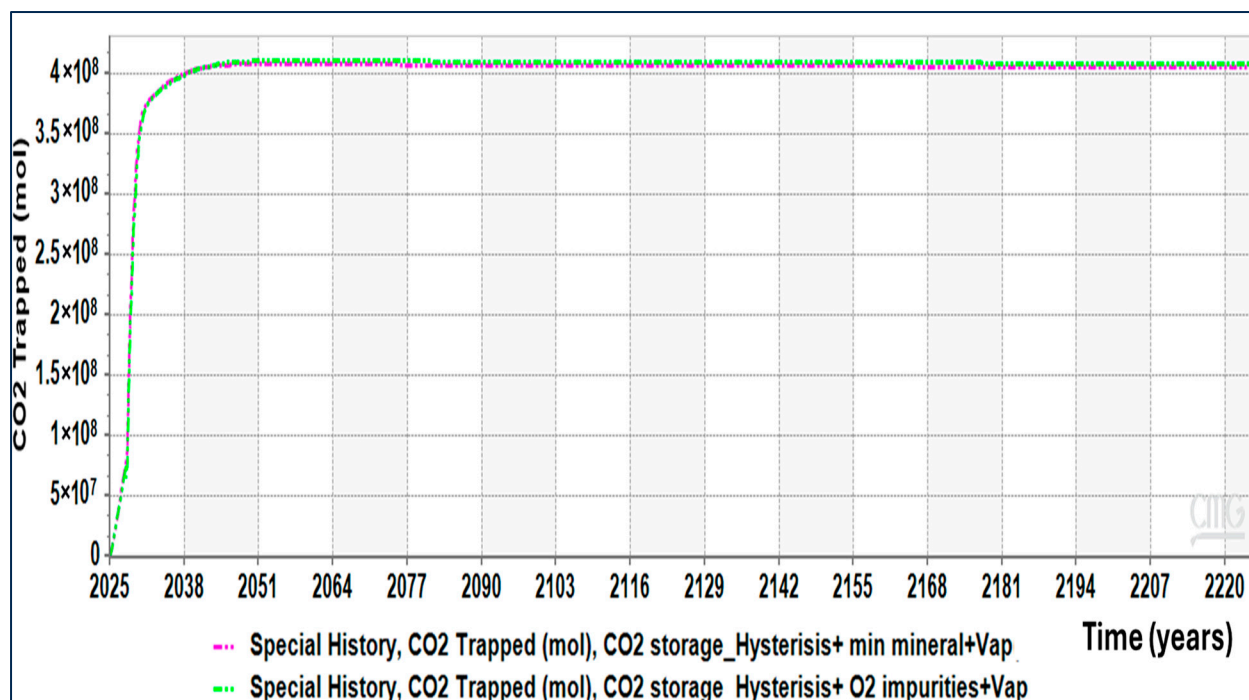
This involves two scenarios, the pure CO₂ stream with processes of hysteresis, mineralization, and vaporization, while the second involves the same gas trapping configuration but incorporates the effect of O₂ impurities. The total mass of the CO₂ injection process has remained more or less the same. But there would be a slight variation in the proportion of different processes. The curves of the two for the trapped CO₂ in Figure 18 would be almost overlapping. This would further reveal that the effect of the presence of oxygen would have less bearing on the migration of the plume. Also, Table 14 shows a comparison between the two cases.

Table 14. The effect of simulating the O₂ impurities.

Component	Without O ₂	With O ₂	Effect
Supercritical CO ₂	Same	Same	No impact on storage capacity
Capillary trapped CO ₂	Same	Same	No impairment
Dissolved CO ₂	Slightly higher	Slightly lower	Competition in aqueous phase

Table 14. Cont.

Component	Without O ₂	With O ₂	Effect
Mineralized CO ₂	Lower	Higher	O ₂ enhances dissolution, releasing more Ca ²⁺ into brine and CO ₂ reacts and converted to minerals
Reservoir pH	Low (more acidic)	Slightly higher pH	Better geochemistry
Overall safety	Stable	Stable	Both are safe

Figure 18. Comparison of CO₂ trapped trend with and without O₂ impurities.

In both examples, the supercritical CO₂ increases dramatically in the 1-year injection phase but falls off very rapidly in the latter phases as the plume evolves into a new equilibrium dominated by residual trapping.

A few decades after shut-in, the level of the supercritical phase has reached a steady-state low but equal value in both examples, verifying that the overall dynamics of plume-scale fluid movement are largely controlled by rock properties, regardless of minute gas composition differences.

More significant disparities exist in the geochemical aspects of gas trapping. A qualitative analysis of the mineralized CO₂ profiles in Figure 19 indicates that the presence of oxygen results in a slightly higher mineral trap capacity over the entire 200-year simulation period. In the scenario without impurities, the mineralized CO₂ concentrations grow very aggressively shortly after the gas injection but taper off subsequently when the most reactive mineral surface sites become exhausted.

With the inclusion of O₂, the mineral CO₂ curve always remains above the base case scenario. This implies that oxygen causes additional mineral dissolution and chemical reaction mechanisms that lead to more divalent ions being released into the brine. These chemical reactions extend for a longer period of carbonate mineral formation. Consequently, a relatively higher portion of the CO₂ becomes trapped in the solid mineral phases. The practical effect of the oxygen-filled stream is the additional push toward the more permanent trap.

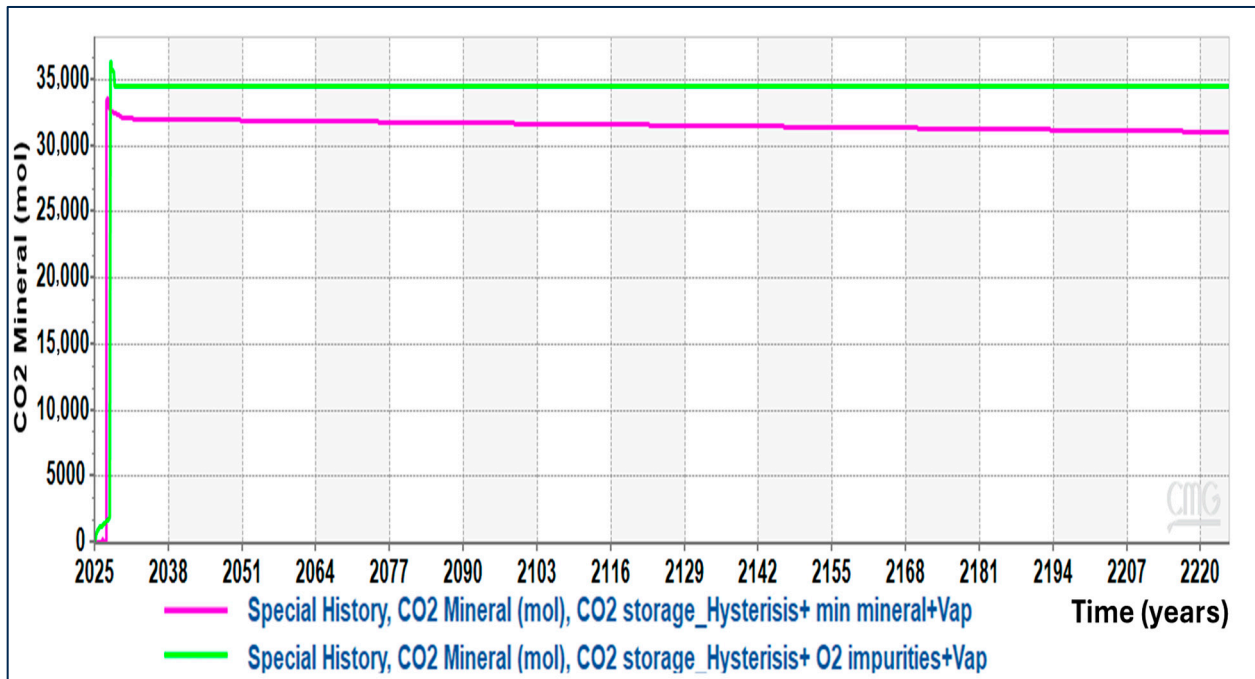


Figure 19. Comparison of CO₂ Mineral trend with and without O₂ impurities.

Figures 20 and 21 show that the figures of dissolved & aqueous ionic CO₂ (molality & carbonate & bicarbonate ions) add to the picture. In both cases, the immediate effect of the injection was a rapid increase in the concentration of dissolved CO₂ in the plume. With the passage of time, however, the figures show a slight variation in the trend of the concentrations of dissolved & ionic CO₂. In the no oxygen case, the concentration remains a bit higher.

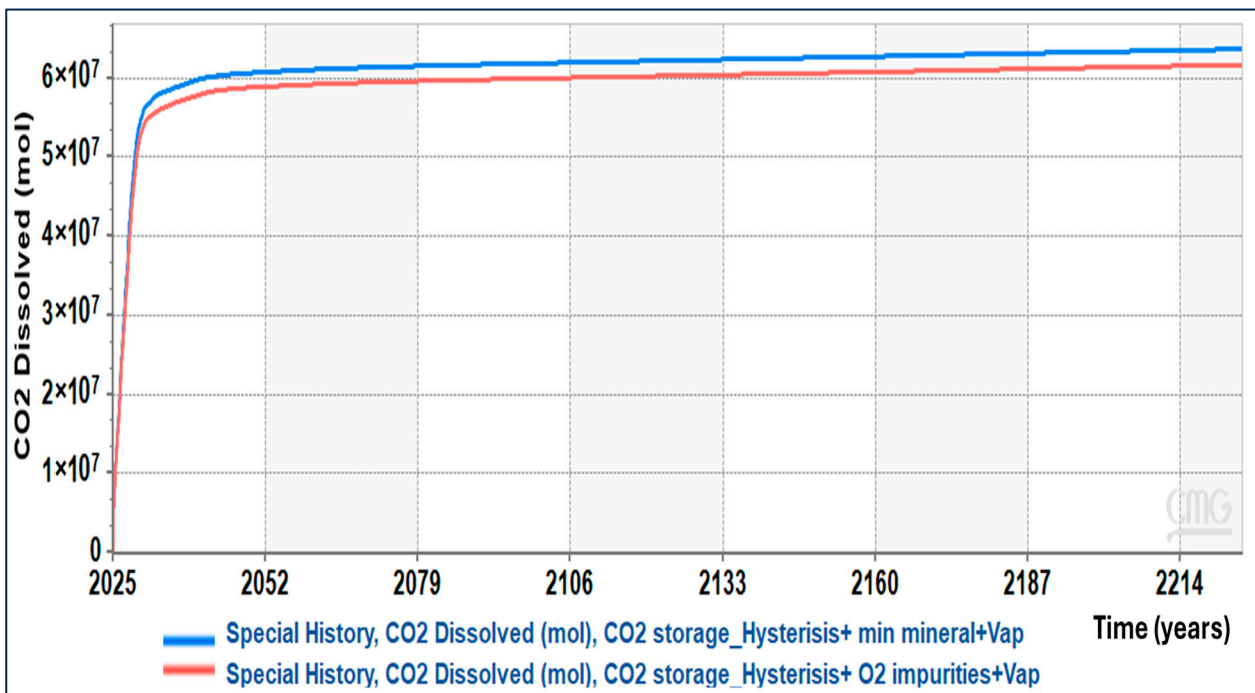


Figure 20. Comparison of CO₂ Dissolved trend with and without O₂ impurities.

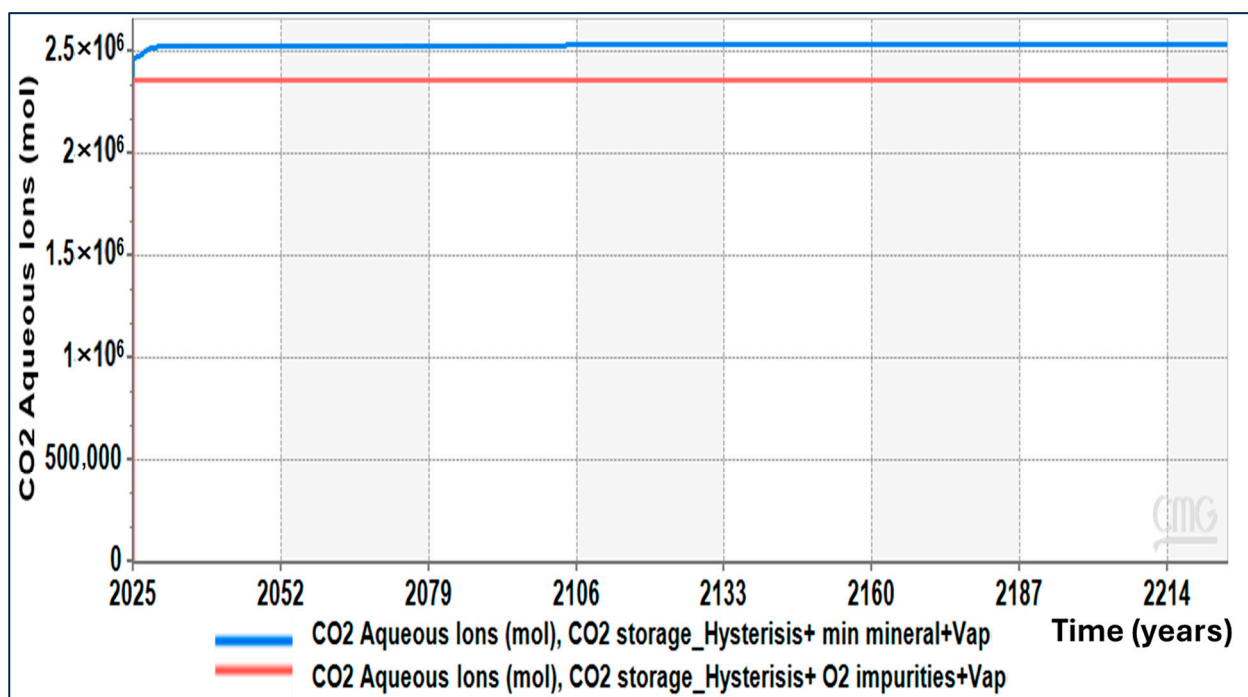


Figure 21. Comparison of CO₂ Aqueous ions trend with and without O₂ impurities.

This occurs in agreement with the higher mineralization present in the O₂ scenario. With the higher conversion of dissolved CO₂ to solid carbonate phases, there will be less remaining in the dissolved form. Essentially, the presence of O₂ does not inhibit the dissolution of CO₂. Instead, the dissolution of CO₂ in the presence of oxygen triggers a faster chemical reaction to remove the dissolved CO₂ into the solid phases.

These trends together indicate that the influence of O₂ impurities on total storage capacity or physical immobilization at the Early Time (Supercritical + Residual) is not significant but affect the distribution of chemically trapped CO₂ between dissolved or ionic form and mineral form. The scenario of pure CO₂ keeps more CO₂ in the dissolved phase, while the scenario of mixtures of CO₂ + O₂ keeps a slightly higher portion of CO₂ in mineral form.

For secure storage, however, the re-partitioning of CO₂ in the form of a change from dissolved CO₂ to solid mineral carbonates is a positive development for storage security because the mineral form of CO₂ will remain in storage permanently. The oxygen-rich stream will therefore induce a small but significant positive effect in terms of the permanence of the trap. Otherwise, the path of the trap remains the same.

4.4. Simulation Running Time

The plot provides an outline of the simulation run times for the CO₂ storage scenarios ordered with respect to increasing run time, demonstrating the cumulative effect of increasing levels of complexity. It should be noted that the simplest scenarios, the “Base” and the “Hysteresis Only” simulation, have the shortest run times because these examples are relatively simple and consist only of basic multiphase fluid dynamics with little or no nonlinear couplings. Within these example scenarios, the migration of the CO₂ is primarily controlled by structural trapping and the system dynamics allow for the use of very large timesteps and fast convergences.

Figure 22 shows the running time of the different scenarios studied. The coupling of mineralization, hysteresis, and vaporization causes a pronounced increase in the runtime. When simulating mineral entrapment, both multiphase flow processes and geochemi-

cal reactions, like aqueous speciation, have to be linked, whereas simulations involving vaporization imply additional phase equilibrium calculations. Despite this complexity, the solver still has to deal with a highly coupled nonlinear problem, which increases computational time.

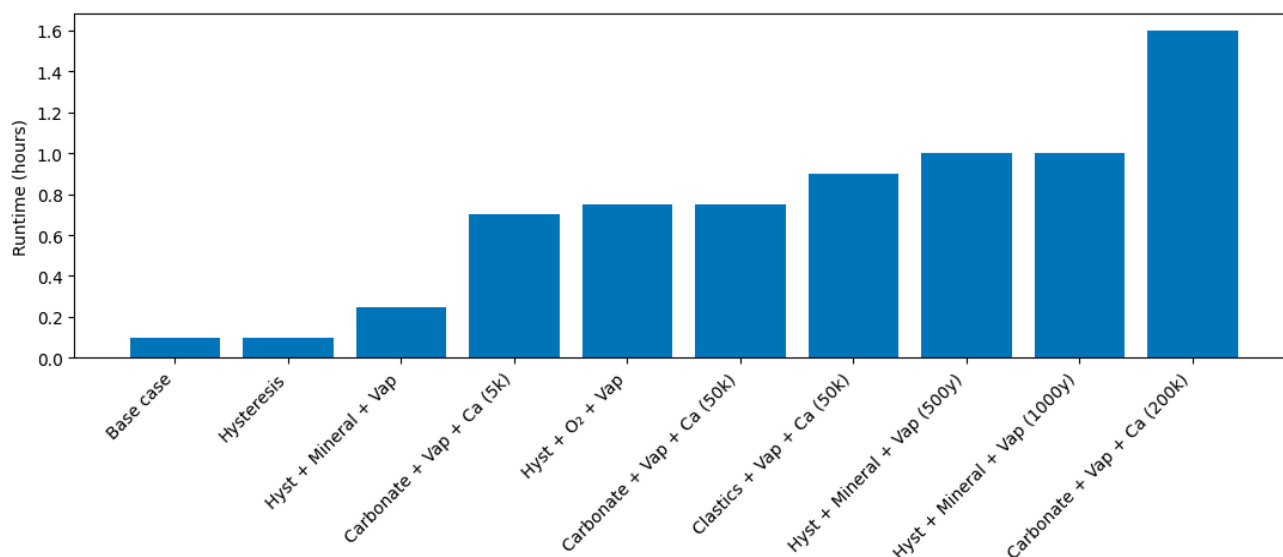


Figure 22. Simulation Runtime comparison for CO₂ storage cases.

Carbonate systems involving vaporization but having low Ca concentration resolution (Ca resolution of 5k) have been found to have intermediate simulation times. It should be noted that although calcium chemistry is simulated at a relatively coarse resolution, reactions involving carbonate minerals remain active. This signifies that even when Ca resolution is very coarse, there is a large computational overhead compared to other physical trapping mechanisms.

The added O₂ species further raises the simulation time due to additional equations for mass balances and the speciation of the aqueous and gas phases. The expanded chemistry scheme introduces numerical stiffness and limits time stepping.

An increase in the Ca concentration solution to a level of 50k in clastic sedimentary geologies, combined with vaporization, leads to a higher runtime. The Ca concentration tracing process increases the species and reactions in the aqueous component, increasing the interaction between the hydrologic transport process and geochemistry. This increases non-linearity and the number of iterations.

The runtime for the systems involving vaporization, Ca, with a concentration of 50k, is slightly higher for the carbonate systems compared to clastic systems. This is expected, as the reactivity of the systems, along with the rock-fluid-chemistry interactions, makes the systems stiffer, even for a moderate level of chemical resolution.

In these cases with intermediate timesteps, the longest running times are those with mineralization, vaporization, and long simulation times of 500 and 1000 years. This is because the long simulations entail more timesteps to account for the slower reactions in mineral trapping, CO₂ dissolution, and geochemical equilibration. This result clearly shows that the effect of simulation time is significant in computationally expensive problems involving geochemistry.

The most computationally intensive problem is the carbonate system with vaporization and high Ca concentration resolution (Ca 200k). In this problem, strongly reactive carbonate minerals, detailed aqueous Ca chemistry, and kinetic discretization all interact to produce a strongly nonlinear and coupled problem. A large number of calculations of chemical

reactions per time step make the problem stiffness and result in the largest runtime as shown above. In particular, the figure shows that there is a tradeoff between physical and geochemical fidelity and speed for simulations involving CO₂ storage.

While structural trapping and hysteresis simulations are computationally inexpensive, mineralization, multi-component phase simulations, simulations involving tracking the Ca concentrations, longer-term prediction, and higher geochemical resolution are runtime intensive. Such findings illustrate the need for appropriate model complexity choices depending on the context of the simulations, especially when performing large-scale sensitivity analyses.

4.5. Future Work and Recommendations

Though this work brings out certain aspects of trade-off and computation cost for CO₂ storage simulations with significant benefit, several important extensions are proposed for improving the realism and applicability of the modeling system.

First, the simulation studies should be extended to simulate depleted hydrocarbon reservoirs. In view of the complexity introduced by the presence of residual hydrocarbon saturation, wettability, depletion, and existing wells, depleted hydrocarbon reservoirs are much more complicated than saline reservoirs. Yet, by simulating depleted hydrocarbon reservoirs, two processes, namely, storage and Enhanced Recovery, can be assessed together.

Secondly, processes of saline precipitation also need to be considered in future modeling exercises. CO₂ injection may cause water vaporization and salt precipitation around injection wells. This could potentially lead to a reduction in porosity and permeability and even loss of injectivity. Modeling processes and mechanisms associated with salt precipitation and dissolution is critical in capturing accurate predictions around injection wells and long-term storage.

Third, facies-controlled geological models with a proper degree of complexity should be used instead of simplified models. The facies-controlled variations in porosity, permeability, mineralogy, and capillary properties are essential for CO₂ plume growth, residual trapping, and geochemical processes. The use of facies models built from seismic information, well logs, and core data would be an important improvement in the simulations of CO₂ storage processes.

In this regard, the incorporation of site-specific static geological models from actual storage formations is highly encouraged. In this respect, site-specific static geological models involve detailed structural frameworks, stratigraphy, faults, as well as mineralization, offering a rather realistic approach for subsurface conditions. Worth noting is the consideration that the computation for actual static geological models is expected to take significant processing time, potentially ranging from many hours to several days. This is brought to light as a realistic consideration for large-scale sensitivity analyses or uncertainty analyses employing fully detailed site-specific static geological data.

Lastly, in light of the high computational expense required for simulations involving high physics and geochemistry, future studies should investigate computational optimization techniques. For example, adaptive meshing, focused activation of geochemical reactions, or hybrid machine learning and simulation flows could be useful techniques to improve computational tractability.

5. Conclusions

This integrated simulation analysis investigates the effect of significant geological and operational factors on the behavior of CO₂ storage over a short-term to long-term simulation period. The results shown in the figures reveal that the combination of the rates of development of different storage mechanisms contributes to overall storage safety. The

major component of the trapped CO₂ is in a supercritical free-phase state directly after the 1-year injection period. A significant redistribution of the gas takes place in the initial decades of storage simulation into immobile phases of CO₂ storage: trapped residual, dissolved, ionic aqueous, and mineral phases. Regardless of the adopted simulation scenario, the long-term migration of CO₂ storage may be dominated by geological processes of chemical transformation of the trapped gas.

A critical observation made in the studies is that the longer the overall simulation period and the longer the duration of the injection of CO₂ (1 year, 10 years, and 50 years) the greater the dissolution and mineralization. This can be attributed to the longer contact between the CO₂ mixture and the rock fluid. This enables the continuous generation of carbonate material in the rock layers. As a result of the continuous generation of carbonate material in the rock layers, the pH falls. Finally, the CO₂ gets trapped in solid form in the rock layers even after a period of 200- to 1000-year simulation.

The mineral composition of the rock exerts a strong influence on the fate of the CO₂. The rock type with a high carbonate content always has a higher concentration of dissolved CO₂, higher pH buffering capacity, as well as a higher degree of mineral trap capacity compared to the elastic rock type. An increase in the surface reactivity of the mineral or the availability of Ca ions (Ca 5000–50,000–200,000 ppm) can subsequently result in the enhancement of CO₂ molality in the dissolution front region.

Capillary trapping effects simulated by hysteresis effects also have a very important role in the simulation. The consideration of hysteresis significantly limits the CO₂ trapped residually. With the consideration of vapor-phase trapping (Vap), further immobilization of CO₂ takes place in a drying-out region around the injection point.

The simulation results for the presence of O₂ impurities in the gas phase, modeling the real gas stream contaminants in the gas capture process, show small but positive effects from the impurities on the geochemistry. Even when the migration of the plume and the trapping factor remain very close to the previous pure CO₂ case, the effect of the presence of O₂ in the gas stream accelerates mineral dissolution reactions significantly. This further increases carbonate precipitation reactions to some extent. For all the scenarios of sensitivity analysis, the key effect is that the proportion of the free-phase (or mobile) CO₂ decreases dramatically to a low level. These results establish the expectation that a qualified site geology profile, including the presence of reactive mineral phases and the conditions of high permeability contrasted with the capability for capillary trapping, can guarantee the long-term storage of CO₂ in a deep-saline aquifer to a very high degree of safety.

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References

1. Bachu, S. Review of CO₂ storage efficiency in deep saline aquifers. *Int. J. Greenh. Gas Control* **2015**, *40*, 188–202. [[CrossRef](#)]
2. Bachu, S.; Gunter, W.D.; Perkins, E.H. Aquifer disposal of CO₂—Hydrodynamic and mineral trapping. *Energy Convers. Manag.* **1994**, *35*, 269–279. [[CrossRef](#)]
3. Golkari, A.; Riazi, M. Experimental investigation of miscibility conditions of dead and live asphaltenic crude oil–CO₂ systems. *J. Petrol. Explor. Prod. Technol.* **2017**, *7*, 597–609. [[CrossRef](#)]

4. Birkholzer, J.T.; Zhou, Q.; Tsang, C.F. Large-scale impact of CO₂ storage in deep saline aquifers—A sensitivity study on pressure response in stratified systems. *Int. J. Greenh. Gas Control* **2009**, *3*, 181–194. [CrossRef]
5. Ampomah, W.; Balch, R.; Cather, M.; Rose-Coss, D.; Dai, Z.; Heath, J.; Dewers, T.; Mozley, P. Evaluation of CO₂ storage mechanisms in CO₂ enhanced oil recovery sites—Application to Morrow sandstone reservoir. *Energy Fuels* **2016**, *30*, 8545–8555. [CrossRef]
6. Bell, J.B.; Shubin, G.R. Higher-order Godunov methods for reducing numerical dispersion in reservoir simulation. In *Proceedings of the SPE Reservoir Simulation Conference, Dallas, TX, USA, 10–13 February 1985*; SPE: Richardson, TX, USA; p. 179.
7. Bennion, D.B.; Bachu, S. Drainage and imbibition relative permeability relationships for supercritical CO₂/brine and H₂S/brine systems in intergranular sandstone, carbonate, shale and anhydrite rocks. *SPE Reserv. Eval. Eng.* **2008**, *11*, 687. [CrossRef]
8. Allis, R.; Chidsey, T.; Gwynn, W.; Morgan, C.; White, S.; Adams, M.; Moore, J. Natural CO₂ reservoirs on the Colorado Plateau and southern Rocky Mountains—Candidates for CO₂ sequestration. In *Proceedings of the 1st National Conference on Carbon Sequestration, Washington, DC, USA, 14–17 May 2001*; US Department of Energy National Energy Technology Laboratory: Albany, OR, USA, 2001.
9. Burnside, N.M.; Naylor, M. Review and implications of relative permeability of CO₂/brine systems and residual trapping of CO₂. *Int. J. Greenh. Gas Control* **2014**, *23*, 1–11. [CrossRef]
10. Bahaa, M.; Shokir, E.; Mahgoub, I. Soft Computation Application: Utilizing Artificial Neural Network to Predict the Fluid Rate and Bottom Hole Flowing Pressure for Gas-lifted Oil Wells. Presented at the Abu Dhabi International Petroleum Exhibition & Conference, Abu Dhabi, United Arab Emirates, 12–15 November 2018. [CrossRef]
11. CSA Z741-12; CSA Group Z741-12 Geologic Storage of Carbon Dioxide: Mississauga, Ontario. Canadian Standards Association: Toronto, ON, Canada, 2012. Available online: <https://www.csagroup.org/store/product/Z741-12/> (accessed on 1 October 2025).
12. Cavanagh, A.J.; Wildgust, N. Pressurization and brine displacement issues for deep saline formation CO₂ storage. *Energy Procedia* **2011**, *4*, 4814–4821. [CrossRef]
13. Delprat-Jannaud, F.; Korre, A.; Shi, J.Q.; McConnell, B.; Arvanitis, A.; Boavida, D.; Car, M.; Gastine, M.; Grunnaleite, I.; Bateman, K.; et al. *State-of-the-Art Review of CO₂ Storage Site Selection and Characterisation Methods*; Korre, A., McConnell, B., Delprat-Jannaud, F., Eds.; CGS Europe Report No. D3.3: September, 116; CGS Europe: Weybridge, UK, 2013; p. 41.
14. Emera, M.K.; Sarma, H.K. Prediction of CO₂ solubility in oil and the effects on the oil physical properties. *Energy Sources Part A* **2007**, *29*, 1233–1242. [CrossRef]
15. Gerard, J. *Stratigraphic Traps—Quantitative Approach Based upon a Producing Field Database: American Association of Petroleum Geologists, Search and Discovery Article #40436*; AAPG Annual Convention: Denver, CO, USA, 2009.
16. Chung, F.T.; Jones, R.A.; Nguyen, H.T. Measurements and correlations of the physical properties of CO₂-heavy crude oil mixtures. *SPE Reserv. Eng.* **1988**, *3*, 822–828. [CrossRef]
17. Shokir, E.M.E.-M.; Hamed, M.M.; Ibrahim, A.-E.S.; Mahgoub, I. Gas lift optimization using artificial neural network and integrated production modeling. *Energy Fuels* **2017**, *31*, 9302–9307. [CrossRef]
18. Akai, T.; Kuriyama, T.; Kato, S.; Okabe, H. Numerical modelling of long-term CO₂ storage mechanisms in saline aquifers using the Sleipner benchmark dataset. *Int. J. Greenh. Gas Control* **2021**, *110*, 103405. [CrossRef]
19. Glazewski, K.A.; Aulich, T.R.; Wildgust, N.; Nakles, D.V.; Hamling, J.A.; Burnison, S.A.; Livers, A.J.; Salako, O.; Sorensen, J.A.; Ayash, S.C.; et al. *Best Practices Manual (BPM) for Site Characterization: Plains CO₂ Reduction (PCOR) Partnership Phase III Draft Task 4 Deliverable D35 for U.S. Department of Energy National Energy Technology Laboratory Cooperative Agreement No. DE-FC26-05NT42592, Grand Forks, North Dakota*; Energy & Environmental Research Center: Grand Forks, ND, USA, 2017.
20. Global CCS Institute. Global Status of CCS | Global CCS Institute. 2025. Available online: <https://www.globalccsinstitute.com/global-status-of-ccs/> (accessed on 1 October 2025).
21. Hamling, J.A.; Gorecki, C.D.; Klapperich, R.J.; Saini, D.; Steadman, E.N. Overview of the Bell Creek Combined CO₂ Storage and CO₂ Enhanced Oil Recovery Project. *Energy Proc.* **2013**, *37*, 6402–6411. [CrossRef]
22. Jin, L.; Bosshart, N.W.; Oster, B.S.; Hawthorne, S.B.; Peterson, K.J.; Burton-Kelly, M.E.; Feole, I.K.; Jiang, T.; Pekot, L.J.; Peck, W.D.; et al. *Bell Creek Test Site—Simulation Report: Plains CO₂ Reduction (PCOR) Partnership Phase III Draft Task 9 Deliverable D66 (Update 5) Executive Summary for U.S. Department of Energy National Energy Technology Laboratory Cooperative Agreement No. DE-FC26-05NT42592, Grand Forks, North Dakota*; Energy & Environmental Research Center: Grand Forks, ND, USA, 2016.
23. Li, S.; Dong, M.; Li, Z.; Huang, S.; Qing, H.; Nickel, E. Gas breakthrough pressure for hydrocarbon reservoir seal rocks—Implications for the security of long-term CO₂ storage in the Weyburn Field. *Geofluids* **2005**, *5*, 326–334. [CrossRef]
24. Peck, W.D.; Anagnost, K.K.; Botnen, B.W.; Botnen, L.S.; Daly, D.J.; Gorecki, C.D.; Grove, M.M.; Harju, J.A.; Jensen, M.D.; Jones, M.L.; et al. *Plains CO₂ Reduction (PCOR) Partnership Atlas*, 5th ed.; Energy & Environmental Research Center: Grand Forks, ND, USA, 2016. Available online: https://pcor.undeerc.org/media/khta0u0x/wdp_d81-task1_pcor_atlas_5thedition_revised_final_sep17.pdf (accessed on 1 October 2025).
25. Marini, L. *Geological Sequestration of Carbon Dioxide—Thermodynamics, Kinetics, and Reaction Path Modeling*; Elsevier: Amsterdam, The Netherlands, 2006; Volume 11.

26. Migliavacca, G. Multi-Energy Static Modeling Approaches: A Critical Overview. *Energies* **2025**, *18*, 1826. [\[CrossRef\]](#)
27. Xu, T.; Apps, J.A.; Pruess, K. Numerical simulation of CO₂ disposal by mineral trapping in deep aquifers. *Appl. Geochem.* **2004**, *19*, 917–936. [\[CrossRef\]](#)
28. Steadman, E.N.; Anagnost, K.K.; Botnen, B.W.; Botnen, L.S.; Daly, D.J.; Gorecki, C.D.; Harju, J.A.; Jensen, M.D.; Peck, W.D.; Romul, L.; et al. The Plains CO₂ Reduction (PCOR) Partnership—Developing carbon management options for the central interior of North America. *Energy Procedia* **2011**, *4*, 6061–6068. [\[CrossRef\]](#)
29. Gorecki, C.D.; Liu, G.; Bailey, T.P.; Sorensen, J.A.; Klapperich, R.J.; Braunberger, J.R.; Steadman, E.N.; Harju, J.A. The Role of Static and Dynamic Modeling in the Fort Nelson CCS Project. *Energy Procedia* **2013**, *37*, 3733–3741. [\[CrossRef\]](#)
30. Mattax, C.C.; Dalton, R.L. Reservoir Simulation (includes associated papers 21606 and 21620). *J. Pet. Technol.* **1990**, *42*, 692–695. [\[CrossRef\]](#)
31. Moore, J.; Adams, M.; Allis, R.; Lutz, S.; Rauzi, S. Mineralogical and geochemical consequences of the long-term presence of CO₂ in natural reservoirs: An example from the Springerville–St. Johns Field, Arizona, and New Mexico, USA. *Chem. Geol.* **2005**, *217*, 365–385. [\[CrossRef\]](#)
32. Wilkin, R.T.; Digiulio, D.C. Geochemical impacts to groundwater from geologic carbon sequestration: Controls on pH and inorganic carbon concentrations from reaction path and kinetic modeling. *Environ. Sci. Technol.* **2010**, *44*, 4821–4827. [\[CrossRef\]](#)
33. Teletzke, G.F.; Lu, P. Guidelines for Reservoir Modeling of Geologic CO₂ Storage. *Energy Procedia* **2013**, *37*, 3936–3944. [\[CrossRef\]](#)
34. Computer Modelling Group Ltd. *WinProp. User Guide—Phase Behavior & Fluid Property Program*. WinProp Fluid Modeling Guide | PDF | Phase (Matter) | Phase Diagram; Computer Modelling Group Ltd.: Calgary, AL, Canada, 2023.
35. Soong, Y.; Goodman, A.L.; McCarthy-Jones, J.R.; Baltrus, J.P. Experimental and simulation studies on mineral trapping of CO₂ with brine. *Energy Convers. Manag.* **2004**, *45*, 1845–1859. [\[CrossRef\]](#)
36. Li, Y.K.; Nghiem, L.X. Phase equilibria of oil, gas and water/brine mixtures from a cubic equation of state and Henry’s law. *Can. J. Chem. Eng.* **1986**, *64*, 486–496. [\[CrossRef\]](#)
37. Ismail, I.; Fotias, S.P.; Pissas, S.; Gaganis, V. Optimized CO₂ Modeling in Saline Aquifers: Evaluating Fluid Models and Grid Resolution for Enhanced CCS Performance. *Processes* **2025**, *13*, 1901. [\[CrossRef\]](#)
38. Szulczewski, M.L.; Hesse, M.A.; Juanes, R. Carbon dioxide dissolution in structural and stratigraphic traps. *J. Fluid Mech.* **2013**, *736*, 287–315. [\[CrossRef\]](#)
39. Computer Modelling Group Ltd. *CMG GEM Manual CMG GEM—CO₂—Injection* | PDF | Petroleum Reservoir; Computer Modelling Group Ltd.: Calgary, AL, Canada, 2023.
40. Hamed, M.; Shirif, E. Sustainable CO₂ Storage Assessment in Saline Aquifers Using a Hybrid ANN and Numerical Simulation Model Across Different Trapping Mechanisms. *Sustainability* **2025**, *17*, 2904. [\[CrossRef\]](#)
41. White, S.P.; Allis, R.G.; Moore, J.; Chidsey, T.; Morgan, C.; Gwynn, W.; Adams, M. Simulation of reactive transport of injected CO₂ on the Colorado Plateau, Utah, USA. *Chem. Geol.* **2005**, *217*, 387–405. [\[CrossRef\]](#)
42. Xu, T.; Apps, J.A.; Pruess, K. Reactive geochemical transport simulation to study mineral trapping for CO₂ disposal in deep saline arenaceous aquifers. *Chem. Phys. Miner. Rocks/Volcanol.* **2003**, *108*. [\[CrossRef\]](#)
43. Xu, T.; Zheng, L.; Tian, H. Reactive transport modeling for CO₂ geological sequestration. *J. Pet. Sci. Eng.* **2011**, *78*, 765–777. [\[CrossRef\]](#)
44. Zerai, B.; Saylor, B.Z.; Matisoff, G. Computer simulation of CO₂ trapped through mineral precipitation in the Rose Run Sandstone, Ohio. *Appl. Geochem.* **2006**, *21*, 223–240. [\[CrossRef\]](#)
45. Xu, T.; Apps, J.A.; Pruess, K.; Yamamoto, H. Numerical modeling of injection and mineral trapping of CO₂ with H₂S and SO₂ in a sandstone formation. *Chem. Geol.* **2007**, *242*, 319–346. [\[CrossRef\]](#)
46. He, M.; Luis, S.; Rita, S.; Ana, G.; Euripedes, V.; Zhang, N. Risk assessment of CO₂ injection processes and storage in carboniferous formations: A review. *J. Rock Mech. Geotech. Eng.* **2011**, *3*, 39–56. [\[CrossRef\]](#)
47. Yao, J.; Chen, Z.; Jiang, C.; Peng, X. An Integrated Numerical Study of CO₂ Storage in Carbonate Gas Reservoirs with Chemical Interaction between CO₂, Brine, and Carbonate Rock Matrix. *Appl. Sci.* **2024**, *14*, 6002. [\[CrossRef\]](#)
48. Morgan, H.; Large, D.J.; Bateman, K.; Hanstock, D.; Gregory, S.P. Potential impacts of oxygen impurities in carbon capture and storage on microbial community composition and activity. *Int. J. Greenh. Gas Control* **2021**, *111*, 103479. [\[CrossRef\]](#)
49. Yu, Y.; Yang, G.; Cheng, F.; Yang, S. Effects of impurities N₂ and O₂ on CO₂ storage efficiency and costs in deep saline aquifers. *J. Hydrol.* **2021**, *597*, 126187. [\[CrossRef\]](#)
50. Wang, J.; Ryan, D.; Anthony, E.J.; Wildgust, N.; Aiken, T. Effects of Impurities on CO₂ Transport, Injection and Storage. *Energy Procedia* **2011**, *4*, 3071–3078. [\[CrossRef\]](#)

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