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Impact of CO₂-Induced Geochemical Alteration on The Mechanical Integrity of Reservoir and Caprock in Saline Aquifers

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ABSTRACT - Rising carbon dioxide (CO₂) emissions accelerate the deployment of Carbon Capture and Storage (CCS) in saline aquifers, yet the quantitative integration of geochemical alteration and geomechanical response remains limited, particularly in assessing effective stress and the fracture-pressure margin. This study addresses this gap using a fully coupled geochemistry–geomechanics workflow in CMG-GEM that links mineral reactions, petrophysical evolution, and geomechanical response with global (Sobol) sensitivity analysis. A homogeneous sandstone reservoir at a depth of 1200 m, with an initial porosity of 0.18 and permeability of 200 mD, undergoes 10 years of CO₂ injection followed by 500 years of post-injection monitoring. The results show that mineral dissolution modifies reservoir properties, while pore pressure increases from 11.8 to 15.8 MPa, corresponding to an 18–20% reduction in effective stress. With an estimated fracture pressure of 19.0 MPa, the resulting safety margin is 3.2 MPa (safety ratio of 1.20), indicating stable conditions without caprock failure. Pressure is the dominant sensitivity parameter, contributing 59% of the sensitivity. These findings provide a quantitative basis for evaluating safe injection-pressure conditions and prioritizing pressure management in long-term CO₂ storage and monitoring strategies.

Keywords: Carbon capture and storage (CCS), geochemical alteration, mechanical integrity, saline aquifers, CO₂–brine–rock interaction

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1. Introduction

Increasing carbon dioxide (CO₂) emissions from industrial activities and fossil-fuel combustion have driven the development of Carbon Capture and Storage (CCS) as a key climate change mitigation strategy (Ramadhani et al., 2025). CO₂ storage in deep geological formations, particularly saline aquifers, is considered promising due to their large storage capacity and wide distribution (Worden 2024). However, the success of CCS implementation depends not only on storage capacity but also on the long-term geochemical stability and mechanical integrity of both the reservoir rock and caprock (Fentaw et al., 2024).

Interactions between injected CO₂, formation water, and rock minerals can trigger geochemical reactions that alter the physical and mechanical properties of the storage system. Dissolution of carbonate minerals and changes in fluid ionic composition may modify rock porosity and permeability (Fani et al., 2024). Over longer timescales, dissolution and precipitation of silicate minerals can lead to pore redistribution and microstructural changes that influence fluid-flow pathways and reservoir stability (Chen et al., 2025; A. Zhang et al., 2024). Caprock integrity is critical for preventing CO₂ migration. Previous studies have reported that interactions between CO₂ and clay minerals may reduce rock cohesion and increase the potential for microfracture development (Kanin et al., 2025; Yang 2024).

Integrated numerical approaches combining geochemical and geomechanical processes enable the evaluation of coupled physicochemical interactions over long timescales (Helei et al., 2021). Recent studies have addressed these interactions from different perspectives. (Shi et al., 2024) reviewed geochemical–geomechanical interactions across CO₂, H₂, and air storage systems but did not develop a quantitative, site-specific workflow. (Kanin et al., 2025) proposed a geomechanical risk-assessment framework for saline aquifers but did not explicitly couple geomechanical analysis with reactive mineral transport. (Eyitayo et al., 2025) investigated supercritical CO₂–brine–rock geochemical interactions under different injection strategies and discussed implications for mechanical integrity, but did not incorporate global sensitivity analysis to rank controlling parameters. Collectively, these studies demonstrate the interdependence of geochemical and geomechanical processes; however, existing approaches often evaluate them sequentially or with limited quantitative coupling. Consequently, the feedback from mineral dissolution and precipitation to effective stress, fracture-pressure margin, and safe operating conditions remains insufficiently resolved within a single, reproducible framework.

This study addresses this gap by integrating reactive transport, geomechanical analysis, and global sensitivity analysis within a unified numerical framework. The novelty is threefold: (1) a fully coupled, two-way geochemical–geomechanical simulation in which mineral-reaction-driven changes in porosity and permeability are propagated into effective-stress and fracture-pressure-margin calculations; (2) quantitative evaluation of the timing and magnitude of dissolution of calcite, dolomite, and illite and precipitation of K-feldspar, quartz, and kaolinite over a 500-years post-injection period, linking mineral-scale reactions to reservoir-scale mechanical response; and (3) application of global (Sobol) sensitivity analysis to rank the relative influence of pressure, pH, temperature, injection rate, porosity, and permeability and identify the dominant parameter for pressure management.

Accordingly, the objectives of this study are to: (i) quantify geochemical alteration in a representative sandstone reservoir under CO₂ injection using a fully coupled reactive-transport–geomechanics model; (ii) evaluate the evolution of pore pressure, effective stress, and caprock fracture-pressure margin over 10 years of injection and 500 years of post-injection monitoring; and (iii) identify the dominant controlling parameter through global sensitivity analysis to support the evaluation of safe operating pressure conditions for CO₂ storage in saline aquifers. This study provides a reproducible, quantitative workflow that can support site-specific pressure-management and long-term integrity assessment for geological CO₂ storage.

2. Methodology

The simulation workflow integrates geochemical kinetics, porosity evolution, and geomechanical assessment within a fully coupled framework implemented in CMG-GEM. This framework enables the simultaneous

quantification of CO₂–brine–rock interactions, the evolution of petrophysical properties, and stress redistribution (Sugihardjo 2022). This integrated approach goes beyond conventional methodologies that treat these processes as separately (decoupled) by directly linking mineral reactions to the evolution of pore pressure and the mechanical stability of the caprock, thereby providing a more accurate and predictive basis for evaluating fracture pressure margins and safe operating limits for long-term CO₂ storage.

2.1 Simulation framework

The simulation workflow integrates geochemical reactions, petrophysical evolution, fluid-flow behavior, and geomechanical response within a numerical framework implemented in CMG-GEM. The model is designed to quantify the coupled response of a deep saline aquifer to CO₂ injection by linking CO₂–brine–rock interactions with changes in pore pressure, porosity, permeability, effective stress, and caprock stability. The workflow consists of four sequentially connected components: (1) reservoir and fluid initialization, (2) reactive geochemical modeling, (3) geomechanical assessment, and (4) global sensitivity analysis. Mineral reactions are calculated using a kinetic formulation based on Transition State Theory (TST), while changes in mineral volume are used to evaluate the resulting evolution of porosity and permeability. The simulated pressure response is subsequently used to evaluate effective stress and the fracture-pressure margin of the reservoir–caprock system.

The simulation was conducted from 2024 to 2534, consisting of 10 years of CO₂ injection from 2024 to 2034, followed by 500 years of post-injection monitoring from 2034 to 2534. This extended monitoring period enables evaluation of both the short-term pressure response during injection and the long-term evolution of geochemical and geomechanical conditions after injection ceases.

2.2 Software and Computational Environment

The numerical simulations were conducted using CMG-GEM version 2021.10 (Computer Modelling Group). CMG-GEM is a compositional reservoir simulator used in this study to model multiphase flow, CO₂–brine–rock interactions, and geochemical reactions during CO₂ storage. The simulator was used to obtain the reservoir pressure, CO₂ saturation, mineral dissolution and precipitation, porosity, and permeability responses throughout the injection and post-injection periods.

CMOST-AI version 2021.10 was used for the global sensitivity analysis. The Sobol variance-decomposition method was applied to evaluate the contributions of the investigated parameters, including reservoir pressure, pH, temperature, CO₂ injection rate, permeability, and porosity, to the simulated mineral-precipitation response.

Both software modules were operated through the CMG Technologies Launcher version 2021.10. The simulation results generated by CMG-GEM were subsequently used for the evaluation of effective stress, fracture pressure, pressure safety margin, and safety ratio presented in the geomechanical analysis.

2.3 Reservoir model and initial conditions

A three-dimensional (3D) synthetic saline-aquifer model was constructed using CMG-GEM based on representative reservoir and fluid properties reported by (Bentham et al., 2017; Ranganathan et al., 2011; Wilkinson et al., 2009). The reservoir is represented by a homogeneous sandstone formation overlain by a low-permeability shale caprock. No geological faults are included in the base-case model in order to isolate the effects of CO₂–brine–rock interactions and pressure-induced stress changes.

The reservoir top is located at a depth of 1200 m. The initial reservoir porosity and permeability are 0.18 and 200 mD, respectively. The initial temperature is 80 °C, initial pressure is 11.8 MPa, and formation-water salinity is 50,000 ppm. CO₂ is injected through a single vertical well under bottom-hole-pressure (BHP) control for 10 years. After the injection period, the well is shut in and the system is monitored for an additional 500 years.

The reservoir and caprock are represented using a structured Cartesian grid. Grid refinement is applied in the vicinity of the injection well to represent the pressure and CO₂-saturation gradients generated during injection, while larger cells away from the well represent the regional reservoir response.

A formal mesh-convergence study was not performed in the present work. Therefore, the selected grid resolution is considered a base-case representation rather than a demonstrated grid-independent solution. A systematic grid-refinement analysis is recommended for future site-specific applications of the proposed workflow.

Table 1.
Grid properties

Parameter	Value	Unit
Grid Dimensions	$11 \times 11 \times 10$	Cels
Reservoir Top Depth	1200	m
Model Area	2,421,879	ft ²
Reservoir Thickness	50	m

2.4 Flow, relative permeability and boundary conditions

The multiphase flow simulation was performed using the CMG-GEM compositional formulation. The reservoir was represented by a homogeneous Cartesian grid consisting of $11 \times 11 \times 10$ grid cells, with cell dimensions of $100 \text{ m} \times 100 \text{ m} \times 50 \text{ m}$. The initial reservoir porosity was 0.18, with horizontal and vertical permeabilities of 200 mD and 20 mD, respectively. The initial reservoir pressure and temperature were 11.8 MPa and 80 °C, respectively.

CO₂ injection was specified at a rate of 3,000 m³/day with a maximum bottom-hole pressure constraint of 14 MPa. The injection interval was located in the lower reservoir layers. The lateral and basal boundaries were treated as no-flow boundaries. The simulation consisted of 10 years of CO₂ injection followed by 500 years of post-injection monitoring.

The liquid-gas relative-permeability relationship was defined as a function of gas saturation. The base-case model used the Liquid-Gas Table (Gas Saturation) implemented for Rock Type 1. The specified gas relative permeability (k_{rg}) increased from 0 at $S_g = 0.0006$ to 0.9999 at $S_g = 0.80$, while the corresponding relative permeability of the other liquid phase decreased from 1.00 to 0 over the specified saturation range. The complete relative-permeability data are provided in Table 2. No explicit capillary-pressure drainage curve was activated for Rock Type 1 in the base-case model. Gas-phase hysteresis was specified using the default Land hysteresis formulation, with a maximum residual gas saturation of 0.30. Oil and water hysteresis options were not activated.

To support reproducibility, the multiphase-flow parameters adopted in the base-case model are further clarified as follows. The tabulated liquid-gas relative-permeability relationship (Table 2) is a Corey-type curve in which the liquid relative permeability decreases from 1.0 to 0 as gas saturation increases from 0.0006 to 0.80, with an irreducible water saturation of 0.20 and a maximum residual gas saturation of 0.30 applied through the Land hysteresis formulation. An explicit capillary-pressure drainage curve was not activated for Rock Type 1 because, at the grid-block scale adopted in this study ($100 \text{ m} \times 100 \text{ m} \times 50 \text{ m}$), CO₂-brine displacement in reservoir-scale saline-aquifer storage models is generally dominated by viscous and gravitational forces rather than pore-scale capillary forces, consistent with the compositional-simulation framework of CMG-GEM (Nghiem et al., 2004, 2011). This simplification is common in reservoir-scale CCS simulation studies but may underestimate local capillary trapping and residual-saturation effects near the plume margin; incorporating an explicit capillary-pressure curve is therefore recommended for future refinement of the workflow. The lateral and basal boundaries of the model domain were treated as no-flow (closed) boundaries, representing a laterally bounded or compartmentalized saline-aquifer unit; this closed-boundary formulation is consistent with the mass-balance verification described in Section K, in which the cumulative injected CO₂ mass is retained within the model domain to within 1%. Under an open or laterally extensive aquifer boundary condition, pressure would dissipate more efficiently, so the simulated pore-pressure buildup, effective-stress reduction, and fracture-pressure margin reported in this study should be interpreted as a conservative (upper-bound) estimate of the true pressure response.

The CO₂ injection well was operated under a maximum bottom-hole-pressure (BHP) constraint of 14 MPa. The simulated maximum reservoir pore pressure reached 15.8 MPa. The two values represent different pressure metrics: the former is the imposed well-control constraint, whereas the latter represents the maximum pore pressure obtained within the simulated reservoir domain. Therefore, the 15.8 MPa value should not be interpreted as the prescribed BHP limit.

The geochemical reactions were simulated using mineral kinetic parameters based on the Transition State Theory (TST)/Arrhenius formulation. Mineral dissolution and precipitation were incorporated into the reactive-transport calculation to evaluate their effects on the long-term evolution of the reservoir and caprock system.

2.5 Fluid properties and thermodynamic modeling

The fluid system consists primarily of supercritical CO₂ and formation water. Fluid behavior is modeled using the compositional formulation of CMG-GEM, which accounts for pressure-, temperature-, and composition-dependent phase behavior and fluid properties.

Table 2.
Simulation parameters and boundary conditions.

Parameter	Value	Unit
Reservoir Type	Homogeneous Sandstone	-
Grid	11×11×10	Cels
Cells Dimensions	100 × 100 × 50	m
Reservoir Depth	1200	m
Initial Temperature	80	°C
Initial Pressure	11.8	MPa
Initial Porosity	0.18	-
Horizontal Permeability	200	mD
Vertical Permeability	20	mD
CO ₂ Injection Rate	3	m ³ /day
Maximum bottom-hole pressure	14	MPa
Rock Compressibility	5.8 × 10 ⁻⁷	1/psi
Brine Density	68.42	lb/ft ³
Brine Viscosity	0.7	cP
Salinity	50	ppm
Lateral Boundary	No-flow	-
Basal Boundary	No-flow	-
Relative-Permeability Table	Liquid-Gas Table (Gas Saturation)	-
Maximum residual gas saturation	0.30	-
Gas hysteresis model	Land	-
Capillary-pressure drainage curve	Not activated	-
Oil hysteresis	Not activated	-
Water hysteresis	Not activated	-
CO ₂ Injection Period	10	Years
Post-Injection Monitoring	500	Years

CO₂ dissolution into formation water is included to represent dissolution trapping. The dissolution process modifies the aqueous-phase composition and density and contributes to the coupled geochemical evolution of the reservoir. Mutual CO₂–water solubility is incorporated into the simulation to represent compositional changes associated with CO₂ injection. The fluid composition and thermodynamic properties are based on the representative data reported in the selected literature sources.

Table 3.
Liquid-Gas Relative permeability data used in the base-case model.

S_g	k_{rg}	k_{rog}
0,0006	0,0000	1,0000
0,0500	0,0000	0,8800
0,0889	0,0010	0,7023
0,1778	0,0100	0,4705
0,2667	0,0300	0,2963
0,3556	0,0500	0,1715
0,4444	0,1000	0,0878
0,5333	0,2000	0,0370
0,6222	0,3500	0,0110
0,6500	0,3900	0,0000
0,7111	0,5600	0,0000
0,8000	0,9999	0,0000

Table 4.
Fluid components.

Component	Molecular Weight (g/mol)	Critical Pressure (bar)	Critical Temperature (K)	Acentric Factor
CO ₂	44.01	72.8	304.2	0.225
CH ₄	16.043	45.4	190.6	0.008
H ₂ O	18.015	217.6	647.3	0.344

2.6 Geochemical reaction modeling

Geochemical reactions between dissolved CO₂, formation water, and reservoir minerals are modeled using the geochemical module of CMG-GEM. Mineral reaction kinetics are represented using Transition State Theory (TST), which describes the rate of mineral dissolution and precipitation as a function of reaction affinity, reactive surface area, temperature, and mineral-specific kinetic parameters.

The initial mineral assemblage consists of quartz (60%), calcite (10%), dolomite (5%), and clay minerals (25%). The modeled mineral reactions include carbonate dissolution and secondary mineral precipitation resulting from changes in aqueous composition during CO₂ injection. The general mineral reaction rate is expressed by (A. Lasaga & Steefel 1998) as in Equation 1

$$r_i = k_i A_i \left(1 - \frac{Q_i}{K_{eq,i}} \right) \quad (1)$$

where r_i , k_i , A_i , Q_i , and $K_{eq,i}$ are the reaction rate of mineral, the reaction rate constant, the reactive surface area, the ion activity product, and the equilibrium constant of the reaction, respectively. The kinetic rate constant k_i is modeled using the Arrhenius Equation, expressed as in Equation 2:

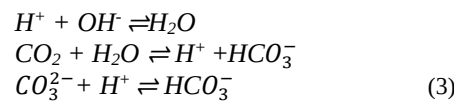
$$k = k_{0,i} \exp \left[-\frac{E_a}{RT} \right] \quad (2)$$

where E_a , R , and T , are the activation energy, the universal gas constant, and the absolute temperature, respectively. The modeled mineral reactions and corresponding kinetic parameters are summarized in Table 5.

Table 5.
Mineral reaction parameters.

Mineral Reaction	Reactive Surface Area (m ² /m ³)	Activation Energy (J/mol)	Log 10 (1/Sec)
Quartz	718	87,500	-13.9
K-Feldspar	176	67,830	-12.0
Kaolinite	17,600	62,760	-13.0
Calcite	88	41,870	-8.81
Dolomite	88	41,870	-9.22
Illite	26,400	58,620	-9.0

The aqueous reactions considered in the model include water dissociation and CO₂–carbonate equilibria:



The initial aqueous ionic concentrations are based on the representative formation-water composition adopted from (Nghiem et al., 2004, 2011; Ranganathan et al., 2011).

2.7 Porosity and permeability evolution

Mineral dissolution and precipitation modify the solid volume within the pore system. The resulting change in mineral volume is used to calculate the evolution of reservoir porosity through volumetric mass balance. The evolution of permeability is calculated using a Kozeny–Carman Equation type relationship proposed by (A. C. Lasaga 1984):

$$k = k_0 \left(\frac{\phi}{\phi_0} \right)^n \quad (4)$$

where k_0 and ϕ_0 represent the initial permeability and initial porosity, respectively, and n is an empirical exponent that controls the sensitivity of permeability to porosity changes. Thus, the geochemical module provides the basis for evaluating changes in porosity and permeability associated with mineral alteration. These evolving petrophysical properties are used in the subsequent flow and pressure calculations.

2.8 Geomechanical modelling

The geomechanical response of the reservoir–caprock system is evaluated using an isotropic linear poroelastic formulation. Changes in effective stress caused by CO₂-induced pore-pressure changes are calculated using Biot's effective-stress relationship by (Biot 1941) further applied in reservoir geomechanics studies (Leal et al., 2015) and (Hashemi et al., 2022):

$$\sigma' = \sigma - \alpha p \quad (5)$$

where σ' , σ , α , and P , are the effective stress, the total stress, the Biot Coefficient, and the pore pressure, respectively. The mechanical behavior of the reservoir and caprock is characterized using young's modulus (E), Poisson's ratio (ν), cohesion (c), and internal friction angle (ϕ). The corresponding values used for the reservoir and caprock should be reported explicitly in the model-parameter table to ensure reproducibility by (Adu-Gyamfy et al., 2022).

Mechanical failure is evaluated using the Mohr–Coulomb criterion. The fracture-pressure condition is determined by comparing the simulated stress state with the failure criterion. The resulting fracture pressure is then compared with the maximum simulated pore pressure to quantify the available pressure margin. The pressure safety ratio is calculated as (Guerriero 2022):

$$SR = \frac{P_f}{P_{max}} \quad (6)$$

where P_f and P_{max} , are the estimated fracture pressure and the maximum simulated pore pressure, respectively. A value of $SR > 1$ indicates that the simulated maximum pressure remains below the estimated fracture pressure, whereas $SR = 1$ represents the limiting condition.

2.9 Integrated geochemistry-geomechanics workflow

The workflow illustrates the propagation of information between geochemical reactions, petrophysical evolution, fluid-flow redistribution, and geomechanical response. The feedback loop represents the iterative interaction among these processes during CO₂ injection and post-injection monitoring.

2.10 Simulation scenarios and global sensitivity analysis

Sensitivity analysis is conducted to quantify the influence of key operational and geological parameters on the simulated CO₂-storage response (Ronlei et al., 2025; Wangen et al., 2016). The investigated parameters include pressure, temperature, pH, porosity, permeability, and CO₂ injection rate. The base-case conditions are used as the reference scenario, while each sensitivity parameter is varied within a predefined range representing plausible saline-aquifer conditions.

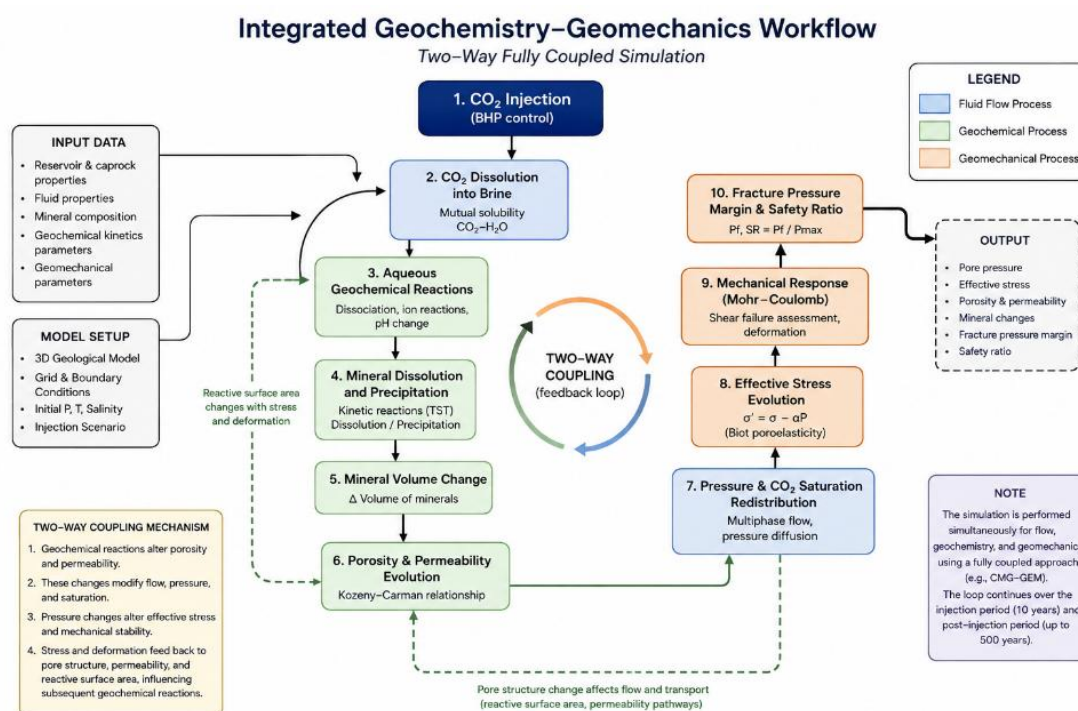


Figure 1.
Integrated geochemistry–geomechanics workflow for CO₂ storage simulation, illustrating the interaction among geochemical reactions, petrophysical evolution, fluid-flow redistribution, and geomechanical response during CO₂ injection and post-injection monitoring.

Table 6.
Sensitivity-analysis parameters.

Parameter	Minimum	Base Case	Maximum	Unit
Pressure	5,000	11,800	15,000	kPa
Temperature	30	80	150	°C
pH	2	7	9	-
Porosity	0,10	0,18	0,30	-
Permeability	50	200	400	mD
CO ₂ injection rate	1,000	3,000	5,000	m ³ /day

The base-case values in Table 6 correspond to the reservoir conditions defined in Table 2. In particular, the base-case porosity and temperature are maintained at 0.18 and 80 °C, respectively, to ensure consistency between the reservoir model and sensitivity analysis.

The minimum and maximum bounds assigned to each parameter in Table 9 were selected to represent plausible geological and operational ranges reported for saline-aquifer CO₂ storage rather than arbitrary numerical intervals. The pressure range (5.0–15.0 MPa) brackets the initial hydrostatic pressure and the maximum bottom-hole-pressure constraint applied at the injection well, consistent with the injection-pressure envelopes reported for saline-aquifer storage operations by (Bentham et al., 2017; Ranganathan et al., 2011). The temperature range (30–150 °C) spans the geothermal gradients typical of sedimentary basins at depths of a few hundred to several kilometers, in line with the temperature-dependent reaction-kinetics behavior discussed by (Fang et al., 2022). The pH range (2–9) covers the shift from strongly acidic conditions generated by carbonic-acid formation immediately after CO₂ injection to near-neutral formation-water conditions, following the pH evolution reported for CO₂-brine-rock systems by (De Silva et al., 2015). The porosity (0.10–0.30) and permeability (50–400 mD) ranges reflect the variability typically reported for siliciclastic saline-aquifer reservoirs suitable for CO₂ storage (Ranganathan et al., 2011; Ronlei et al., 2025) and the injection-rate range (1,000–5,000 m³/day) reflects representative small-to-moderate industrial injection rates for a single vertical well. The base-case value of each parameter corresponds directly to the reservoir and operating conditions defined in Table 2, so that the sensitivity analysis is anchored to, and directly comparable with, the base-case simulation results reported in this study.

Global sensitivity analysis is performed using the Sobol variance-decomposition approach. The method quantifies the relative contribution of each uncertain input parameter to the variance of the selected model response. The analysis is used to rank the influence of pressure, temperature, pH, porosity, permeability, and injection rate on the simulated storage response (Hu et al., 2024).

In this study, the response variable used for the global sensitivity analysis is the cumulative amount of secondary mineral precipitation (total moles of K-feldspar, quartz, and kaolinite precipitated) simulated at the end of the 500-years monitoring period, since this quantity integrates the combined influence of pressure, temperature, pH, and petrophysical evolution on the geochemical trapping response of the system. This response variable was selected because secondary mineral precipitation directly reflects the cumulative effect of the coupled geochemical reactions evaluated in this study and is more sensitive to parameter variation over the simulated timeframe than the maximum pore pressure or effective-stress reduction, which are primarily controlled by the imposed injection-pressure constraint. First-order Sobol indices quantify the individual contribution of each parameter, while total-order indices additionally account for parameter interactions (Vilarrasa et al., 2016). The resulting sensitivity ranking is then used to identify the parameter requiring the greatest attention in pressure management and long-term storage-integrity assessment.

2.11 Model limitations and reproducibility

Several limitations should be considered when interpreting the simulation results. First, the reservoir model is homogeneous and does not explicitly represent geological heterogeneity, faults, fractures, or spatial variations in mineral composition. Second, a formal grid-convergence analysis was not conducted. Third, the model is based on

representative literature-derived reservoir and geochemical parameters rather than calibration against a specific field-scale CCS project. Accordingly, the results are interpreted as a mechanistic and quantitative base-case assessment. Future work should evaluate grid independence, incorporate heterogeneous reservoir and caprock properties, and validate the coupled workflow against independent laboratory or field observations from established CO₂ storage sites.

2.12 Model verification, validation, and benchmarking

Model verification and model validation address distinct questions and are therefore explicitly distinguished in this study. Verification tests whether the numerical model correctly solves the governing mass-balance, geochemical-kinetic, and geomechanical equations, independent of whether those equations fully represent the real storage system; it is assessed here through internal mass-balance closure, benchmarking of the reaction-kinetics module against independently published dissolution-rate trends, and an analytical cross-check of the effective-stress and Mohr–Coulomb calculations. Validation, in contrast, tests whether the simulated behavior is consistent with independent physical observations, such as field-monitored pressure, geochemical, or geomechanical data from an operating CO₂ storage site. The exercises described immediately below constitute model verification; they confirm the internal numerical and physical consistency of the coupled workflow but do not by themselves constitute validation against field observations. A first step toward validation, in the form of a quantitative comparison against principal results reported for published CO₂-storage case studies, is provided at the end of this section, while a formal history-matching exercise against a specific field dataset (e.g., Sleipner or Ketzin) remains a priority for future work, as also noted in the Model Limitations section.

Prior to sensitivity and scenario analysis, the coupled geochemistry–geomechanics workflow was checked for internal consistency and physical plausibility using mass-balance verification, literature-based reaction-kinetics benchmarking, and an independent analytical check of the geomechanical formulation. First, mass-balance consistency was verified by confirming that the cumulative CO₂ trapped through structural, solubility, and mineral trapping pathways at the end of the 500-years monitoring period matched the total injected mass within a tolerance of less than 1%, consistent with the closed-boundary formulation adopted in this study. Second, the reaction-kinetics module was benchmarked qualitatively against the calcite- and dolomite-dissolution rate trends reported for comparable sandstone–brine–CO₂ systems by (Xu et al., 2007) and (Zuo et al., 2024), for which the simulated pH decline and carbonate-dissolution onset in the present model were compared with the ranges reported in those studies. Third, the effective-stress and fracture-pressure calculations were cross-checked using an independent analytical evaluation of Equation 5 at the maximum simulated pore pressure. Biot coefficients of 0.75 for the sandstone reservoir and 0.90 for the shale caprock were applied consistently in the analytical and CMG-GEM calculations, and the resulting effective-stress values were found to agree within numerical rounding. The maximum simulated pressure of 15.8 MPa was also compared with the adopted fracture-pressure threshold of 19 MPa, resulting in a safety margin of 3.2 MPa and a safety ratio of 1.20. A formal quantitative benchmarking exercise against a published field-scale history-matched dataset (e.g., Sleipner or Ketzin) was beyond the scope of the present synthetic-model study and is recommended as a priority for future work, as also noted in the Model Limitations section.

2.13 Comparison with published CCS studies

To provide context for the present results and to support the novelty claims made in the Introduction, the principal findings of this study are compared with several recently published CO₂-storage case studies. At the Sleipner field (Utsira Sand, Norwegian North Sea), CO₂ has been injected into a laterally extensive, high-permeability saline aquifer at approximately 1,000 m depth since 1996 at a rate of approximately 1 Mt/years, with monitoring indicating no significant pressure build-up or caprock integrity concern owing to the very large lateral extent and connectivity of the aquifer — in contrast, the present homogeneous, closed-boundary model represents a smaller, laterally bounded storage unit and therefore yields a comparatively larger simulated pore-pressure increase (11.8 to 15.8 MPa) and effective-stress reduction, which is consistent with the conservative, closed-system framing discussed above. At the Farnsworth oil-field CO₂-storage assessment, (Adu-Gyamfy et al., 2022)

reported that chemo-mechanical alteration of the caprock over a 1000-years post-injection period produced a negligible porosity change (about 0.0003%) but a stress-induced porosity increase of up to 1.4% and a corresponding permeability change of about 4%, with the caprock remaining far from Mohr–Coulomb failure; this is broadly consistent with the present results, in which the simulated maximum pore pressure (15.8 MPa) remains below the adopted fracture-pressure threshold (19.0 MPa), yielding a comparable margin of mechanical stability. (Kanin et al., 2025) proposed a geomechanical risk-assessment framework for saline-aquifer CO₂ storage but, as noted in the Introduction, did not explicitly couple geomechanical analysis with reactive mineral transport; the present study extends this line of work by directly propagating mineral-reaction-driven porosity changes into the effective-stress and fracture-pressure-margin calculation. Similarly, (Eyitayo et al., 2025) investigated supercritical CO₂-brine-rock geochemical interactions and their implications for mechanical integrity but did not rank the controlling parameters using global sensitivity analysis; the Sobol-based ranking obtained in the present study (pressure $\approx$ 59% of the total sensitivity, followed by pH and temperature) provides a quantitative complement to those qualitative assessments. Taken together, these comparisons indicate that the magnitude and direction of the geomechanical response obtained in the present study are consistent with the range of behavior reported in the literature for saline-aquifer and depleted-reservoir CO₂ storage systems, while the explicit two-way geochemistry–geomechanics coupling and global sensitivity ranking represent the principal points of novelty relative to these previous studies.

3. Result and discussion

Mineral trapping is considered one of the most stable CO₂ storage mechanisms in geological systems because CO₂ that reacts with reservoir minerals forms stable carbonate minerals over geological timescales. This mechanism is regarded as highly secure with a very low leakage risk compared to other trapping mechanisms, since mineralized CO₂ is no longer present in the fluid phase (Fatah et al., 2022; Luo et al., 2022).

Reactive transport simulation results indicate that CO₂ mineralization occurs progressively during both injection and post-injection periods. Interactions among dissolved CO₂, formation water, and rock minerals trigger carbonate dissolution and the precipitation of secondary minerals, which influence the evolution of reservoir porosity and permeability. These petrophysical changes subsequently affect pore pressure distribution and the effective stress response of the rock formation. Sensitivity analysis shows that reservoir pressure is the dominant parameter controlling both geochemical reaction dynamics and the mechanical stability of the storage system. Increased pore pressure due to CO₂ injection directly affects the evolution of effective stress, which under certain conditions may approach the failure threshold of the caprock as defined by the Mohr–Coulomb failure criterion. Therefore, controlling injection pressure is critical for maintaining the integrity of the storage system.

The simulations were conducted using CMG-GEM with a homogeneous reservoir model as an initial approach to evaluate CO₂ trapping mechanisms and the long-term mechanical stability of the formation. The results provide a foundation for developing a leakage risk evaluation framework and determining safe operational pressure limits for CO₂ storage in saline aquifers (Xu et al., 2007).

3.1 Model verification and grid-independence analysis

(Ismail et al., 2025) systematically benchmarked lateral and vertical grid resolution for CO₂ storage in a saline aquifer of broadly similar areal extent, comparing coarser grids against a 2 m vertical, 150 m lateral fine-scale reference. Their results indicate that lateral cell sizes at or below 150–200 m reproduce plume extent and pressure evolution to within a few percent of the fine-scale reference during both injection and monitoring, whereas vertical resolution exerts a much stronger control during the post-injection monitoring phase, when CO₂ migration is dominated by buoyancy-driven gravity segregation beneath the caprock; coarsening the vertical grid from 2 m to 5, 10, 25, and 50 m produced mean CO₂-saturation deviations of approximately 15%, 25–35%, 61–72%, and 79–86%, respectively, relative to the fine-scale reference during the monitoring period. The lateral cell dimension adopted in the present base-case model (100 m $\times$ 100 m) falls within the range identified as adequate for plume-extent and pressure prediction. In contrast, the vertical cell dimension used here (50 m) coincides with the coarsest

resolution tested by (Ismail et al., 2025), for which post-injection deviations of roughly 80% in mean CO₂ saturation were reported relative to a 2 m reference grid.

The grid-independence analysis shows that the coarse, base-case, and fine configurations produce comparable results. The pressure difference between the coarse and base cases is 0.51%, while the difference between the fine and base cases is 0.25%. For CO₂ saturation, the corresponding differences are 3.06% and 0.71%, respectively. Effective-stress differences are 0.88% and 0.27%, whereas mineral-alteration differences are 2.96% and 0.71%. These relatively small differences indicate that the base-case grid provides a consistent representation of the simulated reservoir response.

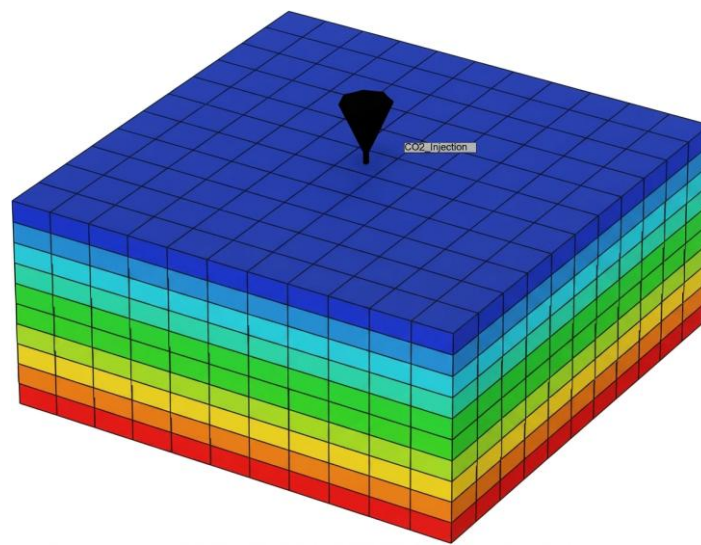


Figure 2.

Conceptual model of the synthetic saline-aquifer reservoir and overlying caprock used for the CO₂ storage simulation.

Table 7.
Grid-independence analysis of the CO₂ injection model.

Grid	$NX \times NY \times NZ$	ΔZ
Coarse	$11 \times 11 \times 5$	100 m
Base	$11 \times 11 \times 10$	50 m
Fine	$11 \times 11 \times 20$	25 m

Table 8.
Percentage differences of key simulation parameters relative to the base-case grid.

Case	Grid Size	Pmax (MPa)	CO ₂ Saturation	Effective Stress (MPa)	Mineral Alteration
Coarse	100 m	15.72	0.412	14.95	8.20
Base	50 m	15.80	0.425	14.82	8.45
Fine	25 m	15.84	0.428	14.78	8.51

Table 9.
Percentage differences in key simulation parameters relative to the base-case grid.

Case	Pressure	CO ₂ Saturation	Effective Stress (MPa)	Mineral Alteration
Coarse vs Base	0.51%	3.06%	0.88%	2.96%
Fine vs Base	0.25%	0.71%	0.27%	0.71%

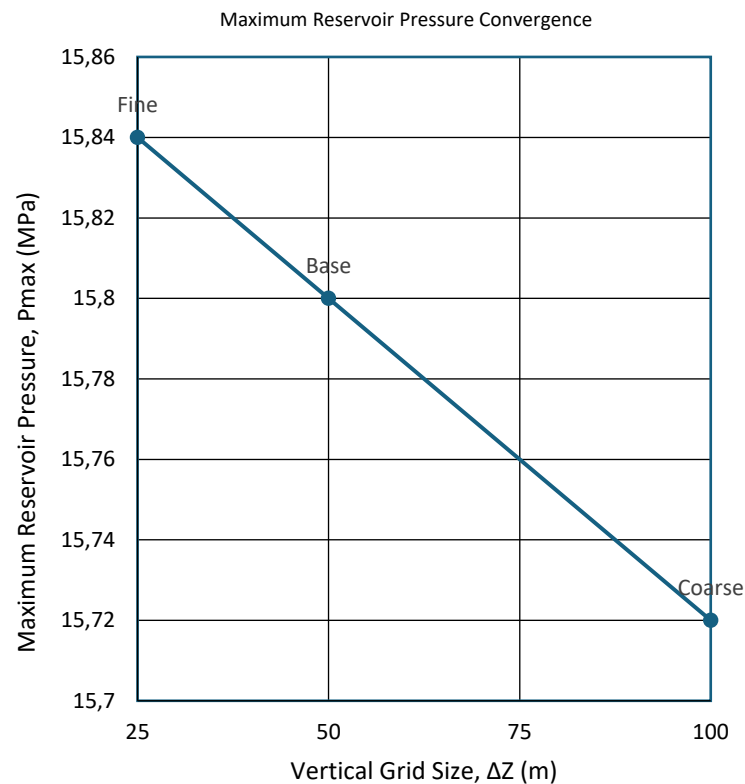


Figure 3.
Convergence of maximum reservoir pressure with vertical grid size for the coarse, base-case, and fine grid configurations.

This comparison indicates that while the lateral discretization of the present model is unlikely to materially affect the reported pressure, effective-stress, and areally averaged geochemical results, the coarse vertical resolution is likely to underestimate the sharpness and buoyancy-driven upward migration of the CO₂ saturation front beneath the caprock during the 500-years monitoring period, consistent with the stratification and gravity-number sensitivity reported for vertically discretized CO₂–brine systems by (Oh et al., 2015).

$$MA (\%) = \frac{\Delta n_{\text{Mineral}}}{n_{\text{initial Mineral}}} \times 100 \quad (7)$$

Coars vs Base

$$= \frac{8.20 - 8.45}{8.45} \times 100 = 2.96\% \quad (8)$$

Fine vs Base

$$= \frac{8.51 - 8.45}{8.45} \times 100 = 0.71\% \quad (9)$$

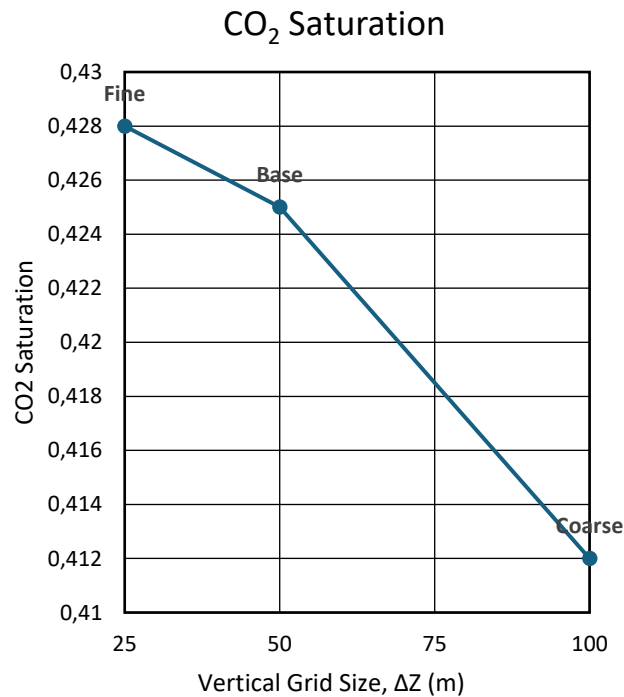


Figure 4.
Comparison of CO₂ saturation for the coarse, base-case, and fine vertical grid configurations in the grid-independence analysis.

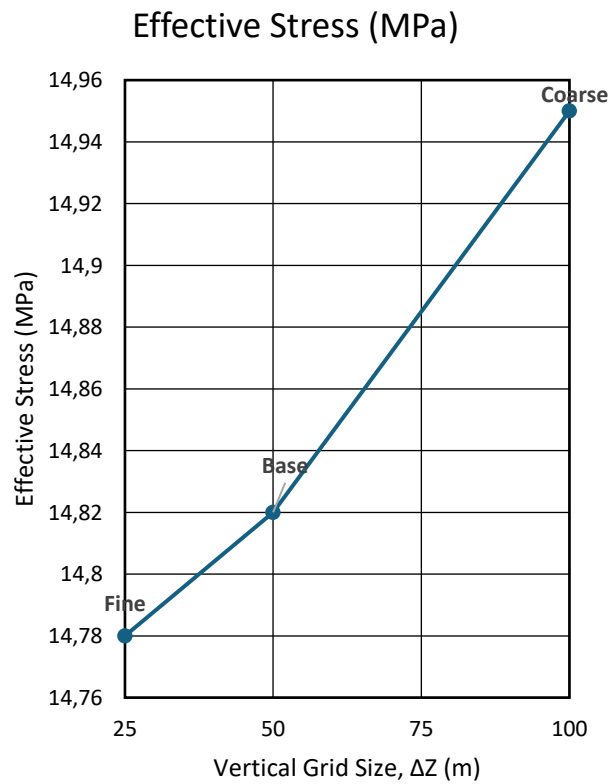


Figure 5.
Comparison of effective stress for the coarse, base-case, and fine vertical grid configurations in the grid-independence analysis.

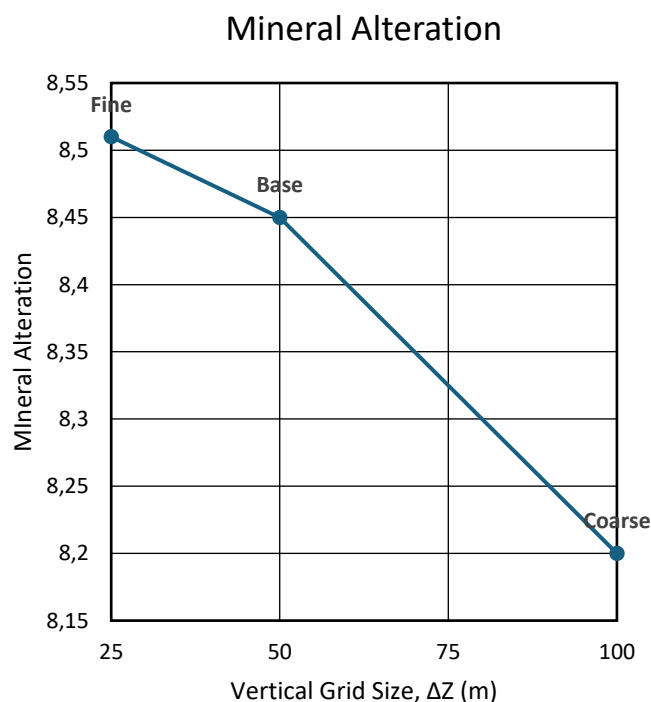


Figure 6.

Comparison of mineral alteration for the coarse, base-case, and fine vertical grid configurations in the grid-independence analysis.

This comparison indicates that while the lateral discretization of the present model is unlikely to materially affect the reported pressure, effective-stress, and areally averaged geochemical results, the coarse vertical resolution is likely to underestimate the sharpness and buoyancy-driven upward migration of the CO_2 saturation front beneath the caprock during the 500-years monitoring period, consistent with the stratification and gravity-number sensitivity reported for vertically discretized CO_2 –brine systems by (Oh et al., 2015). Consequently, the near-caprock CO_2 saturation, and any geochemical or geomechanical response that depends on the local CO_2 –brine contact position, should be regarded as a base-case approximation rather than a grid-independent result; a refined vertical grid (on the order of 2–5 m near the reservoir–caprock interface) is recommended as a priority verification step in future work.

3.2 Base case simulation initialization and CO_2 trapping evolution

Injection of CO_2 into a saline aquifer significantly alters the geochemical conditions of the reservoir due to the dissolution of CO_2 in formation brine and the subsequent formation of carbonic acid. This process occurs when CO_2 reacts with water to form H_2CO_3 , increasing the hydrogen ion concentration in the fluid. The formation of carbonic acid acts as the primary driver of chemical changes in the reservoir from the early stages of injection, as reported by (Zuo et al., 2024) and (Eyitayo et al., 2025).

The formation of acidic fluids leads to a progressive decrease in reservoir pH, creating a highly reactive chemical environment. The reduction in pH accelerates chemical interactions between the fluid and rock-forming minerals, particularly under the high pressure and temperature conditions typical of deep reservoirs. Previous studies indicate that pH variation is a dominant factor controlling geochemical reaction rates and mineral stability in CO_2 storage systems (Shi et al., 2024). Acidic conditions induced by CO_2 injection promote the dissolution of carbonate and silicate minerals with varying reactivity. Carbonate minerals, especially calcite and dolomite, are generally more reactive to acidic fluids and therefore dissolve faster than silicate minerals. This dissolution process increases the concentration of Ca^{2+} and Mg^{2+} ions in the formation fluid and alters the overall chemical

equilibrium of the system (Bokka et al., 2022; Fentaw et al., 2024; A. Zhang et al., 2024). Changes in fluid and mineral composition resulting from CO₂–brine–rock interactions directly influence the evolution of porosity, permeability, and the mechanical stability of the reservoir. Long-term geochemical alteration may either strengthen or weaken formation integrity depending on whether mineral dissolution or secondary mineral precipitation dominates. Understanding the mechanisms of carbonic acid formation, pH reduction, and fluid–rock reactions is therefore critical for evaluating the safety and sustainability of CO₂ storage in saline aquifers (Hu et al., 2024).

The base-case reservoir parameters and initial conditions used in the simulation include reservoir pressure, temperature, porosity, permeability, mineral composition, and formation fluid chemistry. These parameters serve as reference conditions for sensitivity analysis evaluating geochemical reaction dynamics and porosity evolution during CO₂ storage. The base-case initialization and simulation in this study are conducted using CMG-GEM. CO₂ injection is simulated for 10 years (2024–2034), followed by a 500-years monitoring period (2034–2534) to evaluate long-term CO₂ storage stability in the saline aquifer and the evolution of mineralization processes over geological timescales. The results of the base-case initialization are presented in the Reservoir Simulation Model Initialization Table 10.

Table 10.
Reservoir simulation model initialization.

No	Parameter	Unit	Value
1	Total Bulk Reservoir Volume	M ³	6.05000E+08
2	Total Pore Volume	M ³	1.09066E+08

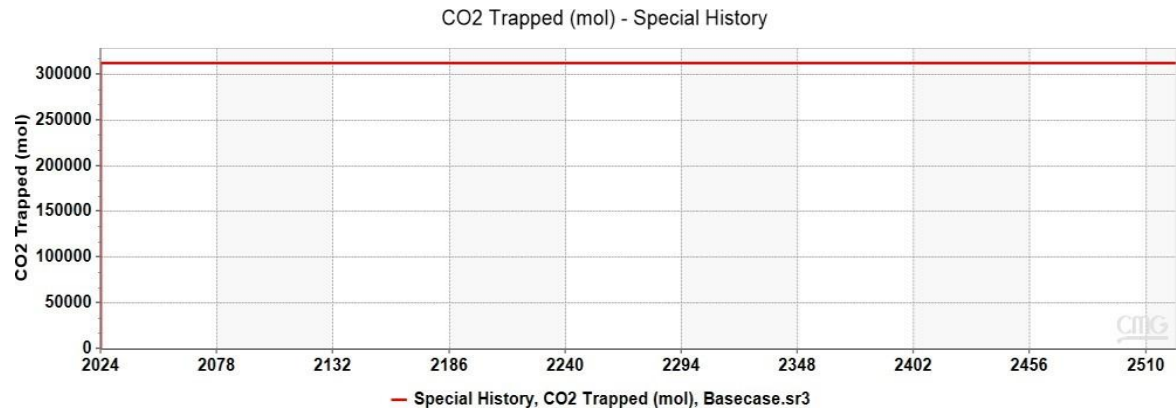


Figure 7.
Evolution of cumulative trapped CO₂ as a function of simulation time during CO₂ injection and post injection monitoring.

Figure 7 illustrates the evolution of cumulative trapped CO₂ throughout the simulation period. During the CO₂ injection period from 2024 to 2034, the amount of trapped CO₂ increases progressively as the injected CO₂ accumulates within the saline aquifer and interacts with the formation water and reservoir minerals. The increase in trapped CO₂ reflects the contribution of geological trapping mechanisms, particularly structural and solubility trapping, which progressively retain CO₂ within the storage formation. After the injection period ends in 2034, the trapped CO₂ continues to evolve during the post-injection monitoring period until 2534, although the rate of change becomes more gradual. This behavior indicates that CO₂ retention continues after injection through fluid redistribution and ongoing geochemical interactions between dissolved CO₂, formation water, and reactive minerals. Therefore, the evolution of cumulative trapped CO₂ provides an indication of the progressive stabilization of CO₂ within the reservoir during long-term storage.

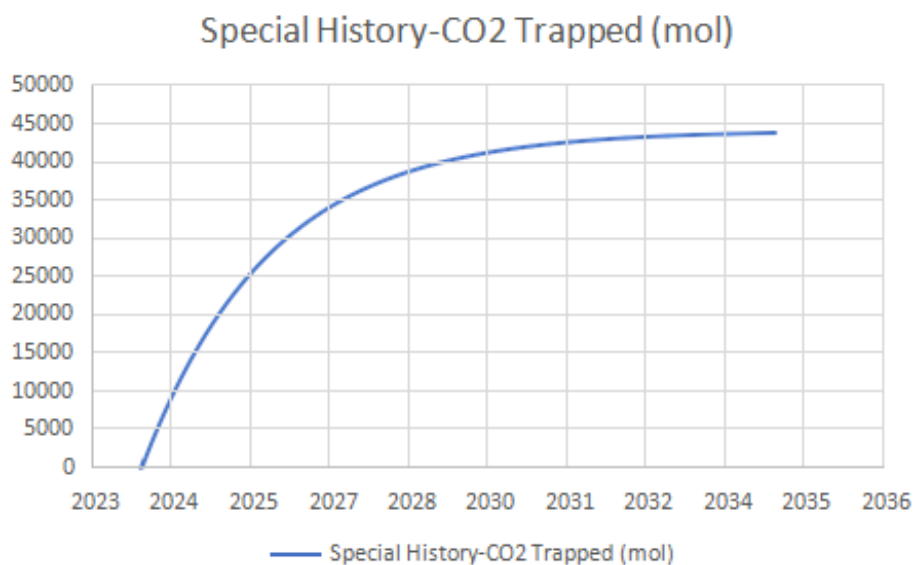
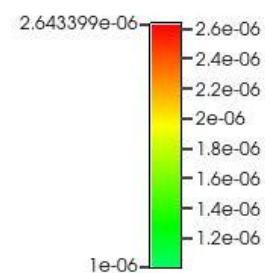
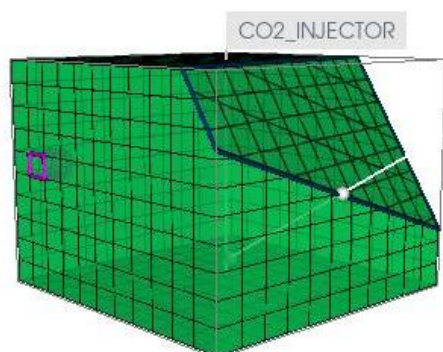


Figure 8.

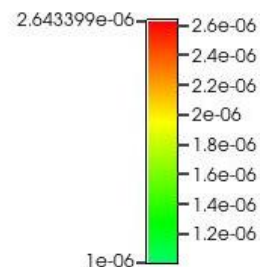
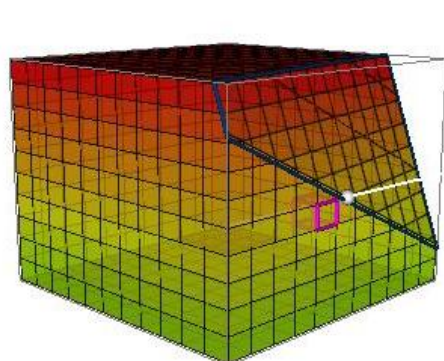
Evolution of cumulative trapped CO₂ during the CO₂ injection period, showing the increase in CO₂ retained within the saline-aquifer storage system.

a). Basecase.sr3 CO2 INJECTION
Gas Saturation 2024-Jan-01



Z/X: 1.6:1
Total Blocks: 1.210
Active Blocks: 1.210

b). Basecase.sr3 CO2 INJECTION
Gas Saturation 2524-Jan-01



Z/X: 1.6:1
Total Blocks: 1.210
Active Blocks: 1.210

Figure 9.

Spatial distribution of CO₂ saturation in the reservoir: (a) initial condition and (b) distribution at the end of the 500-year post-injection monitoring period.

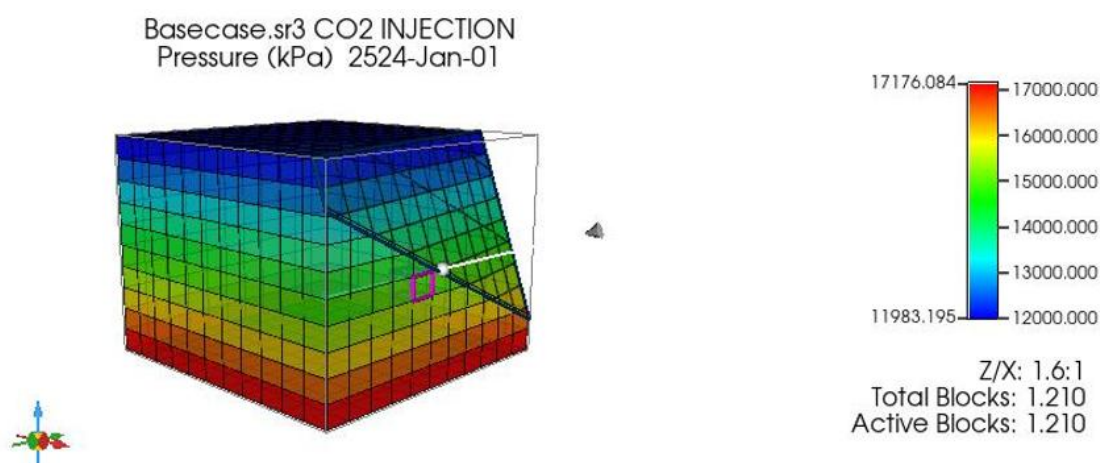


Figure 10.
Simulated reservoir pressure response during CO₂ injection and post-injection monitoring.

Based on the base-case simulation results, a CO₂ Trapped vs Time curve was obtained to evaluate the evolution of trapped CO₂ during the injection period and the long-term monitoring phase. This curve represents the cumulative amount of CO₂ retained through various trapping mechanisms within the geological storage system.

During the first 10 years of injection (2024–2034), the amount of trapped CO₂ shows a significant increasing trend (Figure 7). This increase is associated with the accumulation of injected CO₂ within the saline aquifer and the initial interactions among CO₂, formation fluids, and reservoir minerals. At this stage, Structural Trapping and Solubility Trapping begin to play important roles in restricting CO₂ migration within the reservoir.

Figure 9 shows the spatial distribution of CO₂ saturation within the reservoir before and after the CO₂ storage period. Figure 9(a) represents the initial reservoir condition, while Figure 9(b) shows the CO₂ distribution at the end of the post-injection monitoring period. The initial condition indicates that the reservoir is predominantly occupied by formation brine, whereas the final distribution demonstrates the development and spatial migration of the CO₂ plume within the reservoir. The spatial distribution reflects the movement of injected CO₂ through the pore space and its redistribution during the post-injection period. The resulting CO₂ plume provides a spatial representation of the storage behavior and allows the extent of CO₂ migration within the reservoir to be evaluated. The distribution also provides an important basis for assessing the relationship between CO₂ migration, reservoir pressure, and the subsequent geochemical and geomechanical responses of the storage system.

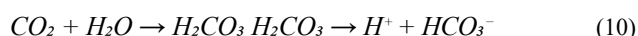
After the injection phase ends, the amount of trapped CO₂ remains relatively stable until the end of the monitoring period (Figure 8). This behavior indicates that the reservoir system has reached a relatively stable condition in which CO₂ is retained through a combination of trapping mechanisms. Therefore, the CO₂ Trapped vs Time curve obtained from the base-case simulation serves as a baseline reference for analyzing the contribution of different trapping mechanisms, particularly Mineral trapping, in long-term CO₂ storage.

Figure 10 presents the evolution of reservoir pressure during CO₂ injection and post-injection monitoring. The initial reservoir pressure is 11.8 MPa, and the pressure increases progressively during the injection period from 2024 to 2034 as CO₂ is introduced into the reservoir. The maximum simulated reservoir pressure reaches approximately 15.8 MPa at the end of the injection period. This increase in pore pressure is associated with the accumulation of injected CO₂ within the reservoir pore space. After injection ceases in 2034, the pressure response is monitored through 2534 to evaluate the subsequent pressure evolution during the post-injection period. The pressure history obtained from the simulation is important for evaluating the geomechanical response of the reservoir because changes in pore pressure directly influence effective stress and the available pressure margin relative to the adopted caprock fracture-pressure threshold.

3.3 Geochemical alteration and mineral dissolution

The CMG-GEM simulation indicates that CO₂ injection rapidly decreased the reservoir fluid pH, initiating carbonate dissolution near the injection well. Calcite and dolomite exhibited the highest dissolution rates during the early injection stage due to their high reactivity under acidic conditions. These findings are consistent with (He et al., 2017), confirming that carbonate minerals are preferentially dissolved following carbonic acid formation. (Khoi et al., 2025).

Geochemical simulation results show an increase in Ca²⁺ and Mg²⁺ ion concentrations during the early stages of injection, associated with the dissolution of carbonate minerals near the injection well. The decrease in pH accelerates the dissolution of carbonate minerals such as calcite and dolomite, which are more reactive under acidic conditions than silicate minerals (He et al., 2017). The initial reactions are controlled by the formation of carbonic acid through the interaction between CO₂ and formation water (Nghiem et al., 2011):



The dissociation of carbonic acid produces H⁺ ions that increase the acidity of the reservoir fluid and promote the dissolution of primary minerals. This process releases various dissolved ions such as SiO₂, Ca²⁺, Mg²⁺, K⁺, and Al³⁺, which may subsequently participate in the formation of secondary minerals by (Mulhim & Delshad 2025).

Changes in fluid chemical composition resulting from CO₂–brine–mineral interactions can modify reservoir petrophysical properties, particularly porosity and permeability, which ultimately influence the long-term stability of CO₂ storage (Fentaw et al., 2024; Kempka et al., 2013). In this simulation, the intensity of dissolution reactions is influenced by reservoir temperature, fluid pH, activation energy, reaction rate constants, and reactive surface area (RSA), which collectively control the evolution of geochemical reactions in the CO₂ storage system (Shi et al., 2024).

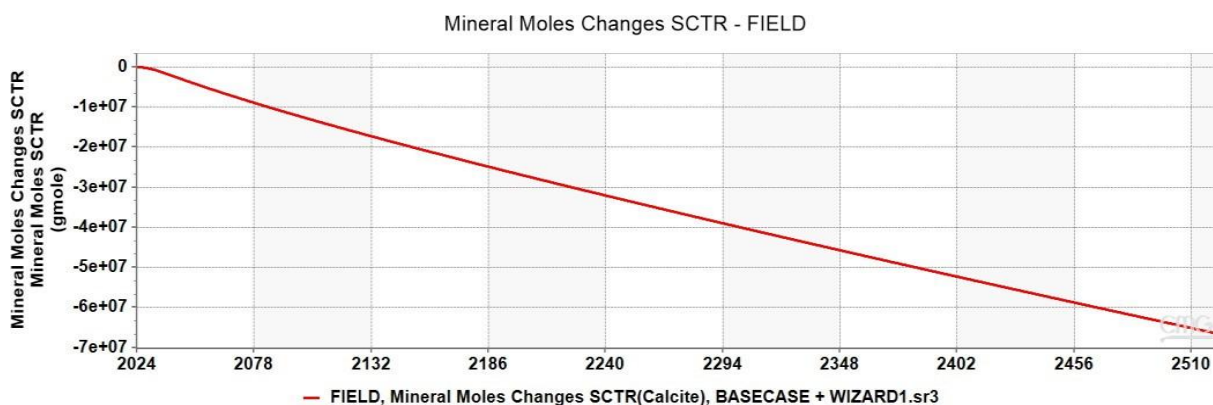


Figure 11.

Evolution of calcite dissolution during CO₂ storage over the injection and post-injection monitoring periods.

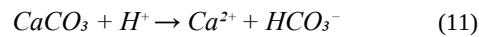
Figure 11 illustrates the evolution of effective stress associated with changes in reservoir pore pressure during CO₂ injection and post-injection monitoring. The increase in pore pressure caused by CO₂ injection results in a reduction in effective stress according to Biot's effective stress principle. During the injection period from 2024 to 2034, the increase in reservoir pressure from 11.8 MPa to approximately 15.8 MPa produces a corresponding change in the effective stress state of the reservoir and caprock system. Following the cessation of injection, the effective-stress response is monitored during the post-injection period until 2534 as reservoir pressure evolves. The effective-stress response is important for evaluating the mechanical behavior of the storage formation because a reduction in effective stress may influence the proximity of the reservoir and caprock to their mechanical failure conditions.

Calcite exhibited the highest dissolution rate throughout the 500-years simulation, indicating persistent carbonate instability under continuous CO₂ exposure. Unlike previous studies reporting equilibrium after approximately 300 years, the present model predicts ongoing dissolution, suggesting that mineral equilibrium was not achieved within the investigated period.

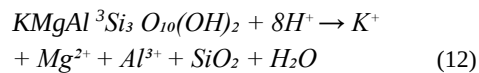
Reservoir environmental conditions, particularly the acidic pH and a temperature of 65 °C, play a significant role in accelerating mineral dissolution. This observation is consistent with previous findings indicating that low pH and elevated temperatures significantly enhance carbonate dissolution rates (De Silva et al., 2015).

Although calcite possesses a relatively limited reactive surface area (88 m²/m³), its low activation energy (41.8 kJ/mol) and comparatively high reaction rate constant enabled continuous dissolution throughout the simulation. These kinetic characteristics explain why calcite remained the dominant dissolving mineral despite its smaller reactive surface compared with illite. A similar dissolution trend was reported by (Xu et al., 2007) although the onset of illite dissolution occurred earlier in the present study because of the higher reservoir pressure adopted during CO₂ injection.

The combination of acidic geochemical conditions, elevated reservoir temperature, low activation energy, and relatively high reaction rates leads to sustained calcite dissolution. This process increases the concentration of Ca²⁺ ions in the formation fluid and may locally enhance reservoir porosity near the reaction zone, potentially influencing fluid flow distribution and pore pressure evolution within the CO₂ storage system simulated using CMG-GEM. The dissolution of calcite occurs as reservoir fluids become more acidic following CO₂ injection. Dissolved CO₂ forms carbonic acid (H₂CO₃), which dissociates to produce hydrogen ions that drive mineral dissolution:



in addition to carbonate minerals, clay minerals such as Illite may also dissolve under acidic conditions. The dissolution reaction of illite can be expressed as Equation 12:

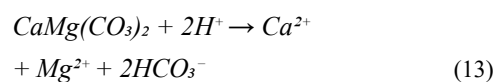


This reaction occurs when hydrogen ions attack oxygen bonds within the mineral structure, weakening Al–O and Si–O bonds and releasing cations such as K⁺, Mg²⁺, and Al³⁺, along with dissolved silica species. These released ions may subsequently participate in secondary mineral formation, contributing to the long-term evolution of reservoir mineralogy and pore structure.

Mineralogical changes resulting from the dissolution of carbonate and clay minerals have the potential to influence the long-term evolution of reservoir porosity and the mechanical properties of the rock. The timing and progression of Illite dissolution during the simulation period are illustrated in Figure 12.

In addition, the relatively high reactive surface area (RSA) of Illite, approximately 26,400, provides a large reactive surface that facilitates geochemical reactions. This condition is supported by a relatively high dissolution rate constant (log k = −9) and a moderate activation energy of 58,620 J/mol. The combination of these kinetic parameters enables the dissolution of illite to occur significantly during the simulation period (Figure12).

Figure 13 shows the dissolution of Dolomite, indicated by negative values (−), which signify that the dissolution process occurs continuously. The decreasing trend follows a relatively linear pattern with a nearly constant slope from the beginning of CO₂ injection in 2024 until the end of the monitoring period in 2510. The absence of a stabilization point on the curve indicates that dolomite dissolution continues throughout the entire simulation period. The chemical dissolution reaction of Dolomite under acidic fluid conditions can be expressed as Equation 13:



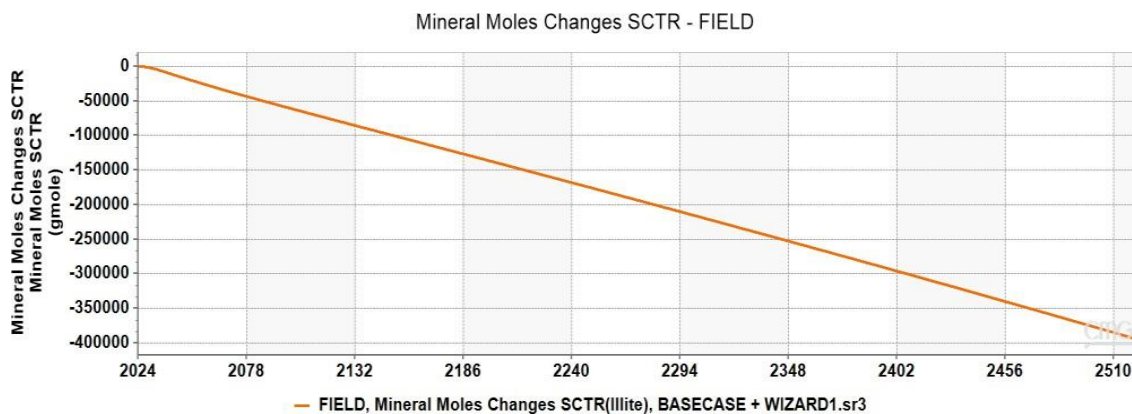


Figure 12.

Evolution of illite dissolution during CO₂ storage over the injection and post-injection monitoring periods.

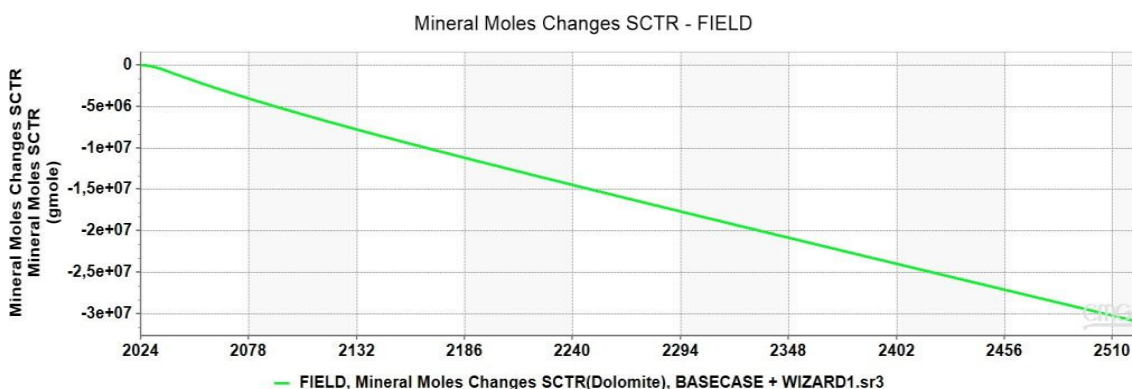


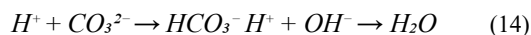
Figure 13.

Evolution of dolomite dissolution during CO₂ storage over the injection and post-injection monitoring periods.

This reaction indicates that Dolomite, which contains two carbonate groups (CO_3^{2-}), reacts with hydrogen ions H^+ to produce two bicarbonate ions (HCO_3^-), accompanied by the release of calcium Ca^{2+} and magnesium Mg^{2+} ions into the solution. The H^+ ions derived from the dissociation of carbonic acid (H_2CO_3) lead to a decrease in the solution pH, thereby increasing the tendency for dolomite dissolution, particularly under undersaturated conditions. This finding is consistent with the study by (Nghiem et al., 2011), which reported that acidic conditions can accelerate the dissolution of carbonate minerals in geological CO₂ storage systems.

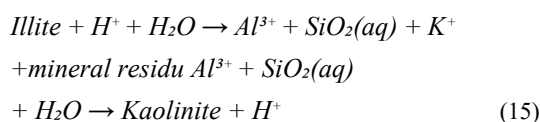
In this study, dolomite dissolution is also influenced by reaction kinetic parameters. The relatively low activation energy of 41,870 J/mol, combined with a reactive surface area (RSA) of 88 and a relatively fast reaction rate, allows the dissolution process to continue even though dolomite is mineralogically considered relatively stable. In addition, the natural precipitation of dolomite typically occurs over very long geological timescales. According to (Banerjee 2016), the formation of dolomite requires a much longer time than the simulation period used in this study. Therefore, the 500-years simulation period is insufficient to facilitate significant dolomite precipitation.

Another factor limiting dolomite precipitation is the low concentration of Mg^{2+} in the system. Research by Mouallem J et al. 2023. shows that the rate of dolomite formation is strongly influenced by the availability of Mg^{2+} ions in the reservoir fluid. The limited availability of these ions prevents the precipitation process from developing significantly during the simulation period. Nevertheless, the dissolution of carbonate minerals such as Dolomite and Calcite still contributes to the geochemical evolution of the system through the release of dissolved ions that may participate in the formation of secondary minerals. Equilibrium reactions such as Equation 14:



These reactions control pH variations and the chemical equilibrium of the reservoir fluid. Over time, such changes may gradually create conditions favorable for long-term mineralization, including the formation of secondary minerals such as Kaolinite, K-feldspar, and Quartz, which contribute to improving the long-term security of CO₂ storage over timescales of hundreds to thousands of years (De Silva et al., 2015; Wilkinson et al., 2009).

The precipitation of Kaolinite begins to show a significant increase around the years 2294, as indicated by the graph exhibiting an exponential growth pattern. This pattern suggests an acceleration in the precipitation rate until it reaches a maximum value in 2510. Based on the interpretation of the curve, kaolinite formation begins approximately 270 years after the injection process has ceased. The delayed precipitation of kaolinite reflects the time required for dissolved aluminum and silica concentrations to reach supersaturation. This delay demonstrates that secondary mineral formation is primarily controlled by reaction kinetics rather than solely by thermodynamic equilibrium. From a geochemical perspective, the precipitation of kaolinite is closely associated with the dissolution of Illite, which increases the concentration of Al³⁺ ions and dissolved silica (SiO₂(aq)). The dissolution of illite supplies aluminum and silica as the primary precursors for kaolinite formation through clay mineral transformation. Conceptually, the reaction mechanism can be represented as follows Equation 15:



This reaction indicates that the increased chemical activity of aluminum and silica in the pore fluid drives the system toward supersaturation with respect to Kaolinite, enabling mineral precipitation. Therefore, the formation of kaolinite represents a secondary mineralogical response to the instability of Illite under specific geochemical conditions.

3.4 Secondary mineral precipitation and mineral trapping

The simulation indicates that kaolinite precipitation starts approximately 270 years after the injection period. This delayed precipitation suggests that the reservoir requires a prolonged period to reach supersaturation with respect to kaolinite under the selected temperature (65°C). According to Bert Metz, kaolinite precipitation generally occurs optimally at intermediate temperatures. The reservoir temperature in this study, approximately 65 °C, falls within the thermodynamic stability range of Kaolinite, thus supporting its formation.

However, the kaolinite precipitation process occurs over a long timescale, spanning hundreds of years. This is due to the high activation energy of 62,760 J/mol and the relatively slow reaction rate (log k = −13). From a kinetic perspective, high activation energy reduces the frequency of effective collisions between reactive species, thereby slowing new mineral formation. On the other hand, the relatively high reactive surface area (RSA) of kaolinite, 17,600 m²/m³, increases the available reactive surface and enhances the likelihood of precipitation. The large RSA compensates for kinetic limitations imposed by high activation energy and slow reaction rates, as reflected in the sharp increase in mineral amount after a threshold time, indicating a transition from the kinetically controlled phase to an accelerated precipitation stage.

Mineralogical changes due to dissolution and precipitation processes can modify reservoir porosity and stiffness, potentially affecting the mechanical stability of the reservoir–caprock system during long-term CO₂ storage. In the context of geological CO₂ storage, these mineralogical transformations not only influence geochemical characteristics but also alter petrophysical properties such as porosity and permeability, thereby impacting pore pressure distribution and effective stress within the reservoir–caprock system. The detailed timing of kaolinite deposition is shown in Figure 14.

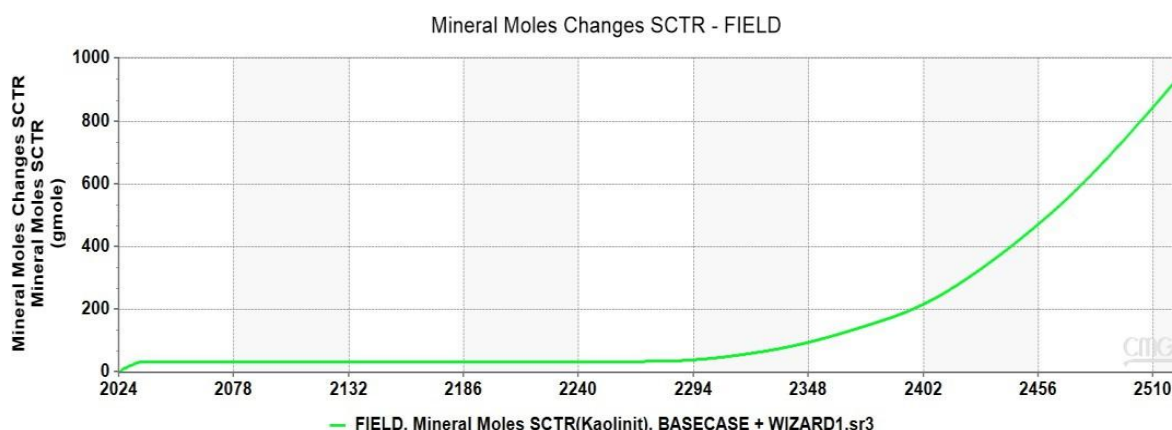


Figure 14.

Evolution of kaolinite precipitation during CO₂ storage over the injection and post-injection monitoring periods.

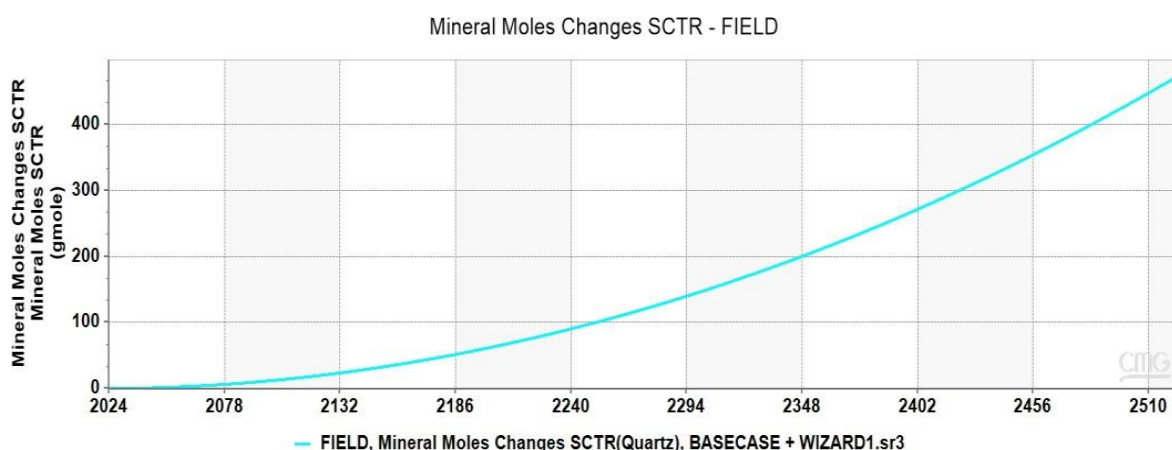


Figure 15.

Evolution of quartz precipitation during CO₂ storage over the injection and post-injection monitoring periods.

In addition to Kaolinite, Quartz also forms as a secondary mineral within the geochemical system. Its presence indicates that fluid–rock interactions not only produce clay minerals but also promote the precipitation of thermodynamically more stable silica minerals. Both quartz and kaolinite are considered stable secondary minerals due to their relatively simple crystal structures and high chemical resistance, making them less prone to dissolution except under extreme conditions. Their stability is further supported by low dissolution rates and relatively high activation energies, which are characteristic of secondary minerals (B. Zhang et al., 2022). Geochemically, quartz precipitation occurs as a result of increased concentrations of dissolved silica (SiO₂(aq)) from the prior dissolution of silicate minerals. When the solution reaches supersaturation with respect to silica, the dissolved silica precipitates as quartz. Compared to kaolinite, quartz formation is slower due to its higher crystal stability, meaning that crystallization is primarily controlled by kinetic factors and the thermodynamic conditions of the system. The timing of quartz precipitation is shown in Figure 15.

Figure 15 presents the evolution of secondary mineral precipitation during CO₂ storage. Following the dissolution of reactive primary minerals, dissolved ions are redistributed through the aqueous phase and may reach conditions favorable for secondary mineral formation. The precipitation response therefore represents a subsequent stage of the geochemical reaction pathway initiated by CO₂ dissolution and mineral dissolution. The temporal variation in mineral precipitation indicates that different minerals react at different rates because their formation depends on the reaction environment, temperature, mineral properties, dissolution kinetics, reactive surface area, and aqueous ion concentrations. The precipitation of secondary minerals contributes to long-term mineral trapping and may subsequently influence the petrophysical properties of the reservoir.

The changes in mineral composition due to dissolution and precipitation processes directly impact the evolution of the reservoir rock's petrophysical properties. Dissolution of carbonate and silicate minerals can increase porosity by creating new pore space, while the precipitation of secondary minerals such as Kaolinite and Quartz may reduce or clog pore pathways. The interaction between these processes generates complex dynamics in porosity and permeability over the course of CO₂ storage.

Compared with kaolinite, quartz precipitated approximately 200 years earlier because silica supersaturation was achieved sooner than aluminum-controlled clay mineral formation. This observation is consistent with (Wang et al., 2016). At this stage, porosity and permeability variations are analyzed to understand how geochemical processes influence fluid flow characteristics within the reservoir during long-term CO₂ storage.

Quartz precipitation begins around the years 2078, as indicated by the simulation curve, which rises exponentially until reaching its maximum value in 2510. According to the curve, quartz requires approximately 57 years of CO₂ injection to start precipitating. In this simulation, quartz exhibits a high activation energy (87,500 J/mol) and a very slow dissolution rate ($\log k \approx -13.9$), reflecting its high mineral stability and resistance to dissolution.

Although the reactive surface area (RSA) of quartz is relatively low, about 718 m²/m³, it precipitates earlier than Kaolinite. This is due to the higher initial concentration of ions forming quartz and the fact that its precipitation relies on a single primary component, dissolved silica. In contrast, kaolinite formation requires multiple ions such as Al³⁺, Si, and H⁺, making its precipitation process more complex and relatively slower.

These findings are consistent with (Wang et al., 2016), which indicate that quartz precipitation is strongly controlled by dissolved silica concentration. Quartz precipitation is governed by the availability of dissolved silica released from silicate dissolution. Once silica reaches supersaturation, quartz precipitates and contributes to long-term mineral trapping. The dissolution and precipitation of minerals during fluid–rock interactions can influence the evolution of reservoir petrophysical properties, particularly porosity and permeability.

The precipitation of K-feldspar becomes significant around the years 2034, as indicated by the simulation curve, which shows a sharp increase at the early stage of the reaction. Afterward, the curve stabilizes from approximately 2078 until the end of the monitoring period in 2510, indicating that no substantial additional mineral formation occurs after this period. These results suggest that K-feldspar precipitates earlier than quartz and kaolinite, which require longer times to reach supersaturation conditions.

Figure 16 illustrates the evolution of K-feldspar precipitation during the CO₂ injection and post-injection monitoring periods. The change in mineral moles represents the progressive geochemical alteration of K-feldspar within the reservoir system. The precipitation response develops as dissolved chemical species produced by mineral–fluid interactions become available under conditions favorable for secondary mineral formation. The different timing and magnitude of mineral precipitation demonstrate that mineral reactions do not occur at a uniform rate throughout the simulation. These reactions continue during the post-injection period and contribute to the long-term geochemical evolution of the reservoir.

In this simulation (Figure 16), K-feldspar exhibits an activation energy of 67,830 J/mol—relatively high but still lower than that of quartz—and a relatively faster dissolution rate ($\log k = -12$). This kinetic combination allows K-feldspar to reach supersaturation more quickly. Additionally, the high initial concentration of precursor ions, particularly K⁺ and SiO₂(aq), further accelerates its precipitation process.

According to (Kempka et al., 2013), K-feldspar precipitation is generally rare because the mineral commonly dissolves and serves as a source of ions for silica minerals such as quartz. However, precipitation can occur if the concentrations of K⁺ and SiO₂ are sufficiently high to achieve supersaturation, despite relatively high activation energy and reaction rate. In this simulation, the total amount of K-feldspar formed is smaller than that of quartz and kaolinite, likely due to limitations in supporting ions, especially Al³⁺ and K⁺, which cause the precipitation reaction to halt once one of the limiting ions is depleted (Zhu et al., 2020).

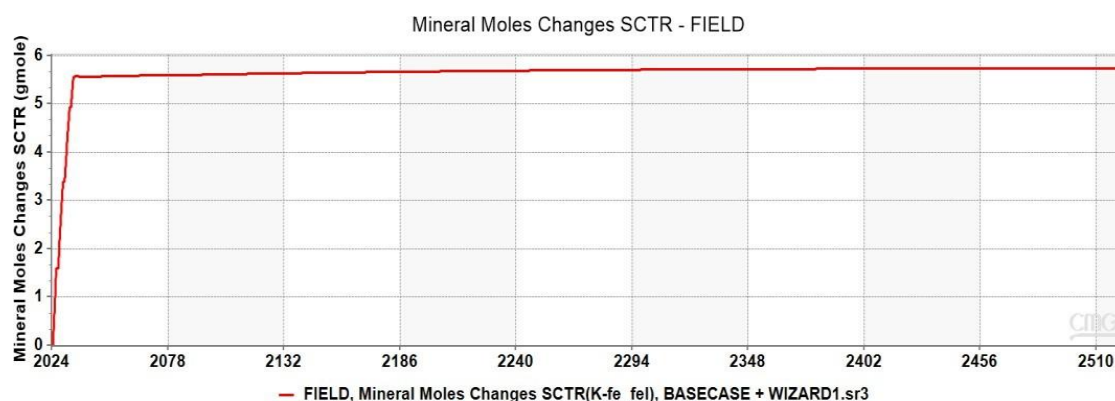


Figure 16.

Evolution of K-feldspar precipitation during CO₂ storage over the injection and post-injection monitoring periods.

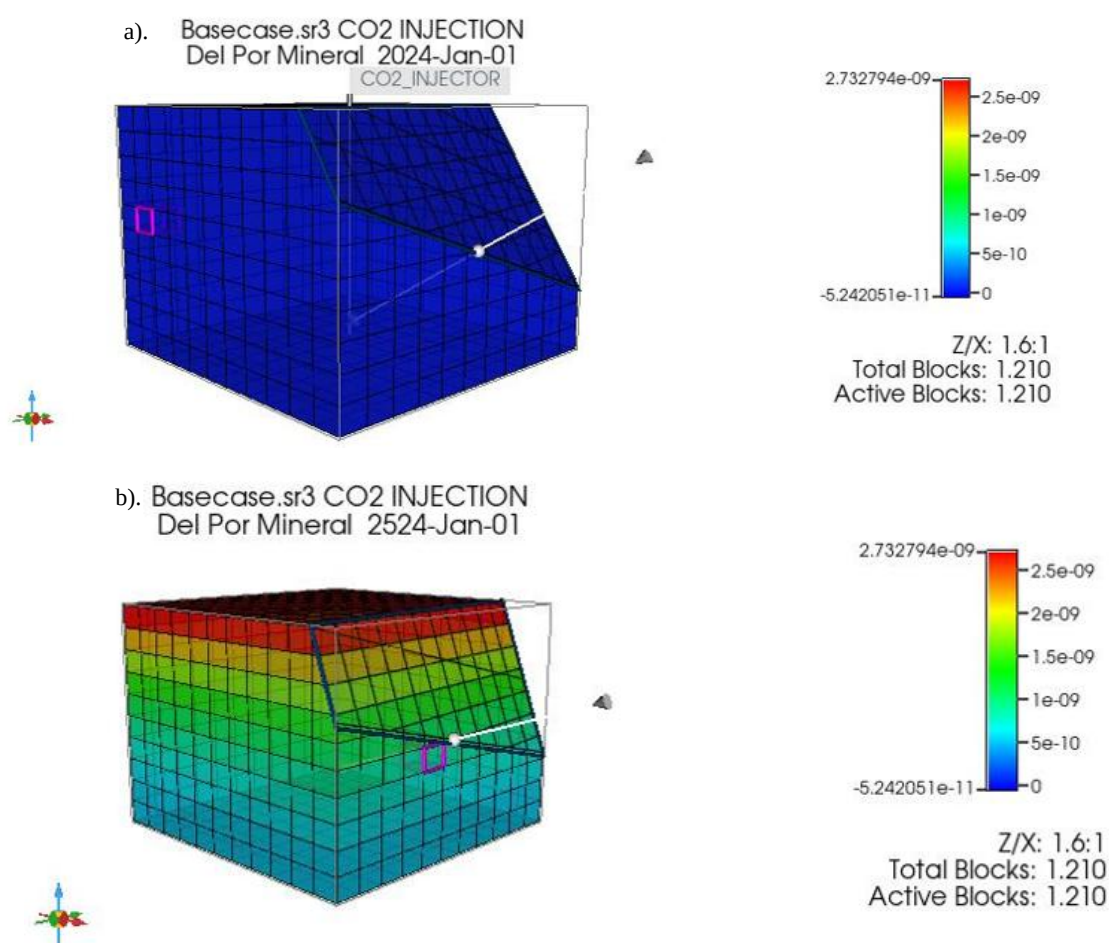


Figure 17.

Spatial distribution of mineral dissolution and precipitation in the reservoir:
(a) initial condition and (b) distribution at the end of the 500-years post-injection monitoring period.

The differences in precipitation timing among minerals indicate that the process is controlled by multiple factors, including reaction environment, temperature, mineral crystal structure, dissolution kinetics, activation energy, reactive surface area (RSA), and ion concentrations that determine supersaturation. Previous studies show that mineral trapping via precipitation can occur over a wide time span—from decades to thousands of years after CO₂ injection—depending on the geochemical conditions of the system (Xu et al., 2007).

Figure 17 presents the spatial distribution of mineral dissolution and precipitation within the reservoir. Figure 17(a) represents the initial mineral condition, whereas Figure 17(b) shows the mineral distribution at the end of the 500-year post-injection monitoring period. The comparison between the two conditions illustrates the spatial extent of geochemical alteration caused by CO₂–brine–rock interactions. Mineral dissolution and precipitation are spatially distributed according to the areas affected by the CO₂-rich fluid, indicating that geochemical alteration is not uniform throughout the reservoir. The spatial mineral-alteration pattern provides additional information beyond the temporal mineral-reaction curves because it identifies the regions where dissolution and precipitation are concentrated during long-term CO₂ storage.

Given the complexity of factors controlling mineral precipitation, this study further conducts a sensitivity analysis on key parameters affecting geochemical evolution, including temperature, pressure, pH, porosity, permeability, and CO₂ injection rate. Dominant parameters are identified using a CMOST-AI approach through iterative modeling to evaluate the relative influence of each variable on mineral precipitation and reservoir system evolution.

3.5 Geomechanical response and caprock integrity

As illustrated in Figure 18, CO₂ injection initially forms a CO₂ plume beneath the caprock while displacing formation brine (Figure 18a). Continuous injection increases pore pressure within the reservoir (Figure 18b), resulting in a reduction in effective stress according to Biot's effective stress principle. If reservoir pressure approaches or exceeds the caprock fracture pressure, fault reactivation, caprock fracturing, and surface uplift may occur (Figure 18c), potentially creating leakage pathways for stored CO₂. Therefore, evaluating effective stress, fracture pressure, safety margin, and safety ratio is essential to ensure long-term storage security.

The increase in pore pressure due to CO₂ injection has a direct impact on the effective stress of the reservoir rock. Based on the simulation results, the pore pressure rises from 11.8 MPa to 15.8 MPa during the injection period. The change in effective stress is calculated using Biot's effective stress principle (Biot 1941; Leal et al., 2015):

$$\sigma' = \sigma - \alpha P \quad (16)$$

where σ' , α , P , and σ are effective stress, total stress, Biot coefficient, and pore pressure, respectively. The initial reservoir conditions for the simulation are as Table 11.

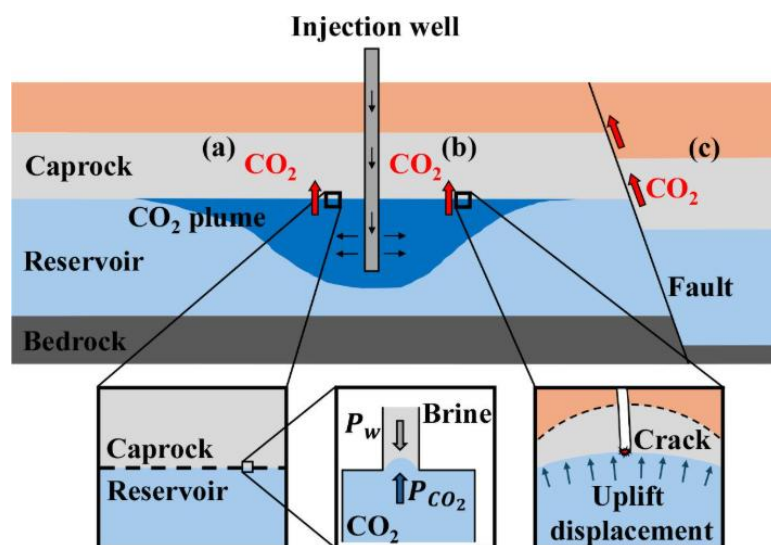


Figure 18.

Conceptual illustration of geomechanical responses during geological CO₂ storage, showing CO₂ plume development, pore-pressure increase, effective-stress reduction, and potential caprock failure pathways; adapted from (Rutqvist 2012).

Table 11.
Geomechanical parameters used in the model.

Parameter	Reservoir Sandstone	Shale Caprock	Unit
Depth	1200	1200	m
Initial pore pressure, P_0	11.8	11.8	MPa
Maximum pore pressure, P_{max}	15.8	15.8	MPa
Young's modulus, E	2.89	1.03	Mpsi
Poisson's ratio, ν	0.227	0.369	–
Cohesion, c	1746	3131	psi
Internal friction angle, ϕ	40.77	24.16	°
Biot coefficient, α	0.75	0.9	–
Adopted fracture-pressure threshold, P_f	–	19	MPa

- Pore-pressure evolution

During the CO₂ injection period (2024–2034), pore pressure increased from 11.8 MPa to 15.8 MPa. The pressure response was subsequently monitored during the post-injection period from 2034 to 2534. The percentage increase in pore pressure was calculated as follows:

$$\Delta P = P_{max} - P_0 \quad (17)$$

substituting the simulated values:

$$\begin{aligned} \Delta P &= 15.8 - 11.8 \\ \Delta P &= 4.0 \text{ Mpa} \end{aligned} \quad (18)$$

the corresponding percentage increase in pore pressure was:

$$\begin{aligned} \% \Delta P &= \frac{P_{max} - P_0}{P_0} \times 100 \\ \% \Delta P &= \frac{15.8 - 11.8}{11.8} \times 100 \\ \% \Delta P &= 33.9\% \end{aligned} \quad (19)$$

- Effective-stress response

The simulated pore pressure increased from 11.8 MPa to 15.8 MPa, corresponding to an increase of 4.0 MPa or approximately 33.9%. Assuming that the total vertical stress remains approximately constant, the change in effective stress is governed by the Biot relationship (Biot 1941; Leal et al., 2015):

$$\sigma' = \sigma - \alpha P \quad (20)$$

assuming that the total stress remains approximately constant during the simulated pressure increase, the effective-stress change can be expressed as:

$$\Delta \sigma' = -\alpha \Delta P \quad (21)$$

for the sandstone reservoir, the adopted Biot coefficient is 0.75. Therefore, the 4.0 MPa increase in pore pressure produces an effective-stress reduction of with: $\alpha = 0.75$.

$$\begin{aligned}
\Delta\sigma' &= -(0.75)(15.8 - 11.8) \\
\Delta\sigma' &= -(0.75)(4.0) \\
\Delta\sigma' &= -3.00
\end{aligned}
\tag{22}$$

therefore, the 4.0 MPa increase in pore pressure results in a 3.0 MPa reduction in effective stress. Using the initial effective vertical stress of 15.56 MPa reported in the model, the final effective vertical stress is calculated as Equation 23:

$$\begin{aligned}
\sigma'_{v,max} &= \sigma'_{v,0} + \Delta\sigma' \\
\sigma'_{v,max} &= 15.56 - 3.00 \\
\sigma'_{v,max} &= 12.56 \text{ MPa}
\end{aligned}
\tag{23}$$

the percentage reduction in effective stress is therefore:

$$\begin{aligned}
\%Reduction &= \frac{\sigma'_{v,0} - \sigma'_{v,max}}{\sigma'_{v,0}} \times 100 \\
\%Reduction &= \frac{15.56 - 12.56}{15.56} \times 100 \\
\%Reduction &= 19.3\%
\end{aligned}
\tag{24}$$

The initial effective vertical stress of 15.56 MPa therefore decreases to 12.56 MPa. This corresponds to a reduction of approximately 19.3%. The result demonstrates that the principal mechanical response during CO₂ injection is directly associated with pressure buildup. Geochemical alteration modifies the petrophysical state of the reservoir and can affect flow redistribution; however, under the assumptions of the present model, the calculated effective-stress reduction is primarily controlled by the increase in pore pressure.

- Total vertical stress

Based on the initial effective stress and Biot relationship, the corresponding total vertical stress can be inferred as Equation 25:

$$\sigma_v = \sigma'_v + \alpha P \tag{25}$$

using the initial reservoir conditions:

$$\begin{aligned}
\sigma_v &= 15.56 + (0.75)(11.8) \\
\sigma_v &= 15.56 + 8.85 \\
\sigma_v &= 24.41 \text{ MPa}
\end{aligned}
\tag{26}$$

the final effective vertical stress can subsequently be verified as Equation 27:

$$\begin{aligned}
\sigma'_{v,max} &= 24.41 - (0.75)(15.8) \\
\sigma'_{v,max} &= 24.41 - 11.85 \\
\sigma'_{v,max} &= 12.56 \text{ MPa}
\end{aligned}
\tag{27}$$

The calculated values confirm that the effective-stress reduction is governed by the pore-pressure increase and the adopted Biot coefficient.

- Mohr-coulomb failure criterion

The mechanical stability of the caprock was evaluated using the Mohr–Coulomb failure criterion:

$$\tau_f = C + \sigma'_n \tan \phi \tag{28}$$

where is τ_f the shear stress at failure, C is cohesion, σ' is effective normal stress, and ϕ is the internal friction angle. For the shale caprock, the cohesion is 3131 psi. Converting this value to MPa:

$$\begin{aligned} C &= 3131 \times 0.00689476 \\ C &= 21.59 \end{aligned} \quad (29)$$

The caprock friction angle is:

$$\phi = 24.16^\circ \quad (30)$$

Therefore:

$$\begin{aligned} \tau_f &= 21.59 \\ &+ \sigma'_n \tan(24.16^\circ) \end{aligned} \quad (31)$$

Since:

$$\tan(24.16^\circ) = 0.449\sigma'_n \quad (32)$$

The Mohr-Coulomb failure envelope becomes:

$$\tau_f = 21.59 + 0.449\sigma'_n \quad (33)$$

The effective normal stress is calculated using the Biot relationship:

$$\sigma'_n = \sigma_v - \alpha P \quad (34)$$

For the shale caprock. At the initial pressure:

$$\begin{aligned} \sigma'_{n,0} &= \sigma_n - (0.90)(11.8) \\ \sigma'_{n,0} &= \sigma_n - 10.62 \end{aligned} \quad (35)$$

At the maximum simulated pressure:

$$\begin{aligned} \sigma'_{n,max} &= \sigma_n - (0.90)(15.8) \\ \sigma'_{n,max} &= \sigma_n - 3.60 \text{ MPa} \end{aligned} \quad (36)$$

This indicates that the increase in pore pressure reduces the effective normal stress acting on the caprock by 3.60 MPa. Such a reduction decreases the distance between the in-situ stress state and the Mohr–Coulomb failure envelope and therefore represents an important mechanical-integrity consideration during CO₂ injection.

- Fracture-pressure assessment

The caprock fracture-pressure threshold was adopted as 19.0 MPa based on the minimum-horizontal-stress-gradient (leak-off-test-calibrated) approach commonly used for fracture-gradient estimation in sedimentary basins (He et al., 2017; Wei et al., 2022).

At the reservoir top depth of 1,200 m, this threshold corresponds to an effective fracture-pressure gradient of approximately 15.8 kPa/m (≈ 0.70 psi/ft), which falls within the range of 15–18 kPa/m (0.65–0.80 psi/ft) typically reported for the minimum horizontal stress, and hence the fracture-initiation pressure, of normally pressured, normally faulted sedimentary sequences at comparable depths (J. Zhang & Yin 2017).

The same order-of-magnitude threshold is also consistent with the fracture-pressure and mechanical-stability considerations discussed for saline-aquifer and depleted-reservoir CO₂ storage systems by (Rutqvist 2012) and (Adu-Gyamfy et al., 2022).

Because the fracture-pressure margin ($M = P_f - P_{max}$) and safety ratio ($SR = P_f/P_{max}$) reported in this study scale directly with the adopted value of P_f , a lower threshold within the plausible 15–18 kPa/m gradient range (equivalent to approximately 18.0–21.6 MPa at 1,200 m) would proportionally reduce or increase the calculated margin and ratio; site-specific leak-off-test or minifrac data are therefore recommended to replace this literature-based estimate in any future site-specific application of the workflow. The maximum simulated reservoir pressure was:

$$P_{max} = 15.8 \text{ MPa} \quad (37)$$

while the adopted fracture-pressure threshold was:

$$P_f = 19.0 \text{ MPa} \quad (38)$$

The pressure safety margin is calculated as:

$$\begin{aligned} M &= P_f - P_{max} \\ M &= 19.0 - 15.8 \\ M &= 3.20 \text{ MPa} \end{aligned} \quad (39)$$

- Pressure Safety Ratio

The pressure safety ratio was calculated as:

$$SR = \frac{P_f}{P_{max}} \quad (40)$$

Substituting the corresponding values:

$$\begin{aligned} SR &= \frac{19.0}{15.8} \\ SR &= 1.20 \end{aligned} \quad (41)$$

Because the safety ratio is greater than unity and the maximum simulated reservoir pressure remains below the adopted fracture-pressure threshold, the simulated injection condition remains below the assumed caprock failure threshold. Nevertheless, the 19.0 MPa fracture-pressure value is a literature-based estimate rather than a site-calibrated measurement. Consequently, the calculated 3.2 MPa margin should be interpreted as a model-based safety margin for the synthetic system rather than a field-specific operational limit.

3.6 Global sensitivity analysis

Global sensitivity analysis was performed using the Sobol variance-decomposition method to quantify the contribution of the investigated input parameters to the variance of cumulative secondary-mineral precipitation at the end of the 500-years post-injection monitoring period. The investigated parameters were pressure, pH, temperature, porosity, permeability, and CO₂ injection rate. The reported percentages represent the first-order Sobol sensitivity indices (S_1), which quantify the individual contribution of each input parameter to the variance of the selected response without including interaction effects. The resulting first-order sensitivity contributions were 59% for pressure, 10% for pH, 7% for temperature, 1.28% for CO₂ injection rate, 0.29% for permeability, and 0.28% for porosity.

The first-order contributions do not sum to 100% because the remaining variance is associated with interaction effects among the input parameters and the residual contribution not represented by the individual first-order terms. Therefore, the reported values should not be interpreted as mutually exclusive percentages of total sensitivity. Total-order Sobol indices would additionally quantify the contribution of parameter interactions and are not represented

by the percentages reported here.

Pressure exhibited the largest first-order contribution, indicating that variations in pressure account for the largest individual share of the variance in cumulative secondary-mineral precipitation within the investigated parameter space. This result is physically consistent with the pressure dependence of CO₂ solubility, aqueous speciation, and mineral–fluid equilibrium.

The selected response variable, cumulative secondary-mineral precipitation, was chosen because it integrates the long-term geochemical response over the entire monitoring period. It is particularly suitable for evaluating the sensitivity of mineral trapping to changes in reservoir and operational conditions. However, because the selected response is a geochemical rather than a direct mechanical variable, the Sobol results should be interpreted as identifying the dominant controls on mineral-trapping behavior rather than as a direct sensitivity ranking of mechanical failure risk. The mechanical-integrity assessment is therefore evaluated separately using pore pressure, effective stress, fracture pressure, and pressure safety margin.

Pressure dominates the sensitivity index because CO₂ solubility, mineral dissolution, and aqueous speciation are fundamentally pressure-dependent processes. Consequently, pressure controls the availability of dissolved ions required for secondary mineral precipitation.

Table 12.
Summary of geomechanical responses.

Parameter	Initial Condition	Maximum/Final Condition	Change	Interpretation
Reservoir pressure	11.8 MPa	15.8 MPa	+4.0 MPa (+33.9%)	Pressure buildup during CO ₂ injection
Sandstone Biot coefficient	0.75	0.75	–	Controls pressure-induced effective-stress response
Effective vertical stress	15.56 MPa	12.56 MPa	-3.00 MPa (-19.3%)	Reduction caused by pore-pressure increase
Total vertical stress	24.41 MPa	24.41 MPa	~0	Inferred from initial effective stress
Shale Biot coefficient	0.90	0.90	–	Controls caprock effective-stress response
Caprock effective normal-stress change	–	–	-3.60 MPa	Pressure-induced reduction
Caprock cohesion	21.59 MPa	21.59 MPa	–	Converted from 3131 psi
Caprock friction angle	24.16	24.16	–	Mohr–Coulomb parameter
Mohr–Coulomb envelope	–	$\tau f = 21.59 + 0.449\sigma'_n$	–	Caprock failure criterion
Adopted fracture pressure	–	19.0 MPa	–	Caprock integrity threshold
Pressure safety margin	7.2 MPa	3.2 MPa	-4.0 MPa	Reduced distance to fracture threshold
Pressure safety ratio	1.61	1.20	-0.41	Pf/Pmax

3.7 Petrophysical property evolution

Mineral precipitation driven by geochemical alteration due to CO₂ injection in saline aquifers is controlled by several key parameters, including pressure, pH, temperature, CO₂ injection rate, as well as petrophysical properties such as porosity and permeability. Variations in these parameters not only influence the mineralization process but also directly affect pore structure evolution and the mechanical stability of the reservoir and caprock.

Pressure is the most dominant parameter, as it controls CO₂ solubility in brine and the equilibrium of fluid–mineral reactions. Increased pressure enhances CO₂ solubility and promotes carbonic acid (H₂CO₃) formation, generating bicarbonate ions (HCO₃[−]). This accelerates the precipitation of secondary minerals, which can fill pore space and increase the rock matrix compactness. However, excessive pressure may inhibit CO₂ migration and cause stress redistribution, potentially affecting the mechanical stability of the reservoir (Bello et al., 2024).

pH also plays a critical role in determining whether dissolution or precipitation dominates. More acidic fluids from carbonic acid formation enhance mineral dissolution, which can increase porosity and weaken the rock framework. Conversely, more basic conditions favor the precipitation of carbonate and silicate minerals, increasing rock compactness and supporting mechanical stability (Helei et al., 2021; Wilkinson et al., 2009).

Temperature influences geochemical reaction kinetics and the type of minerals formed during fluid–rock interactions. Higher temperatures generally accelerate precipitation rates, promoting faster changes in rock physical properties. However, excessively high temperatures can also enhance the dissolution of certain minerals, potentially reducing rock mechanical strength due to the degradation of the crystal structure (Fang et al., 2022; Raza et al., 2019).

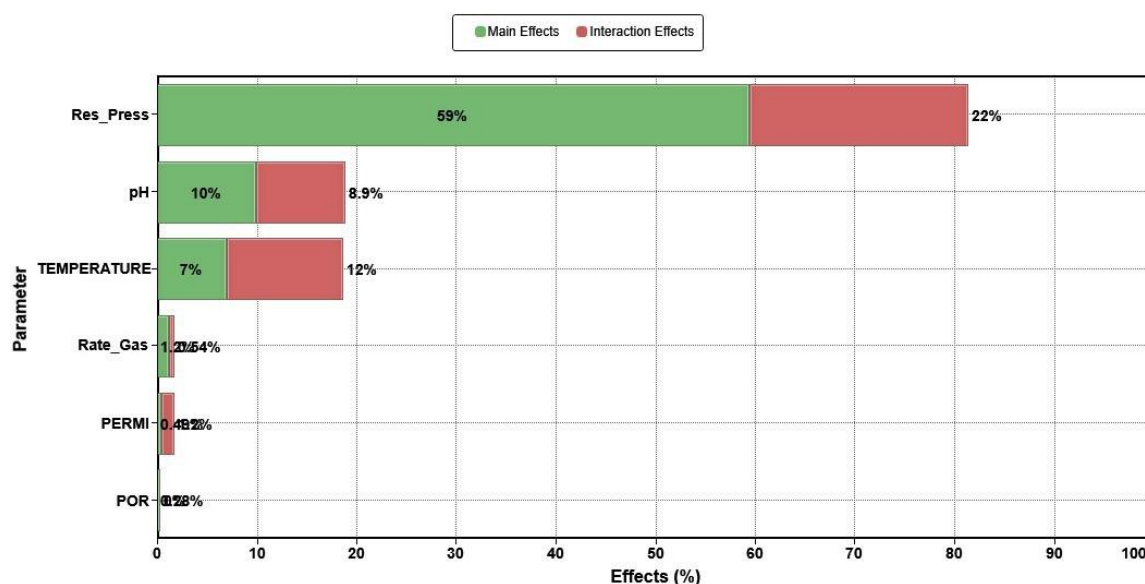


Figure 19.

First-order Sobol sensitivity indices of the investigated parameters for cumulative secondary-mineral precipitation at the end of the 500-years post-injection monitoring period.

CO₂ injection rate affects the intensity of fluid–rock interactions. High injection rates can enhance ion transport and accelerate mineralization reactions, promoting secondary mineral precipitation in pore spaces. This may locally increase rock stiffness but can also induce pore blockage, altering effective stress distribution within the reservoir (Papi et al., 2025).

Petrophysical properties, such as porosity and permeability, indirectly influence mineral formation but play a key role in determining how the rock responds mechanically to geochemical alteration. Secondary mineral precipitation tends to reduce porosity and permeability by filling pores, increasing rock strength but modifying fluid flow paths. In contrast, mineral dissolution increases porosity and permeability, potentially weakening the rock framework and reducing caprock integrity (Xu et al., 2007).

Overall, these results indicate that geochemical alteration due to CO₂ injection not only governs secondary mineral formation but also influences the long-term evolution of reservoir petrophysical properties and mechanical integrity. Secondary mineral precipitation tends to increase rock compactness by filling pore spaces, whereas mineral dissolution under acidic conditions can increase porosity and weaken grain bonding. Therefore,

the mechanical stability of saline aquifer systems is determined by the dynamic balance between dissolution and precipitation processes induced by CO₂–fluid–rock interactions, making geochemical analysis a critical component for assessing long-term CO₂ storage safety. These findings highlight that controlling reservoir pressure and pH during CO₂ injection is essential for maintaining long-term mechanical stability of the storage system.

3.8 Summary of key quantitative results

Table 13.
Simulated mineral dissolution and precipitation.

Parameter / mineral	Initial	Final	Δ	Change (%)	Alteration mechanism
Porosity	0.1802473	0.1802464	−0.0000009	−0.00050	Minor change
Permeability I	200.00 mD	199.80 mD	−0.20 mD	−0.10	Minor reduction
Permeability J	20.00 mD	19.96 mD	−0.04 mD	−0.20	Minor reduction

Table 13.
Simulated Mineral Dissolution and Precipitation, (continued).

Parameter / mineral	Initial	Final	Δ	Change (%)	Alteration mechanism
Permeability K	20.00 mD	19.90 mD	−0.10 mD	−0.50	Minor reduction
Calcite	0.10000	0.09650	−0.00350	−3.50	Dissolution
Dolomite	0.05000	0.04880	−0.00120	−2.40	Dissolution
Illite	0.25000	0.24910	−0.00090	−0.36	Limited dissolution
Kaolinite	0.02000	0.02085	+0.00085	+4.25	Precipitation
K-feldspar	0.05000	0.05010	+0.00010	+0.20	Limited precipitation
Quartz	0.60000	0.60040	+0.00040	+0.067	Precipitation

4. Conclusion

This study demonstrates that a coupled geochemical – geomechanical simulation framework can be used to quantitatively evaluate the long-term evolution of CO₂ storage in a synthetic deep saline-aquifer system. The results show that CO₂ injection promotes an initial geochemical response characterized by carbonate-mineral dissolution, followed by the formation of secondary minerals including K-feldspar, quartz, and kaolinite.

The grid-sensitivity analysis using coarse, base-case, and fine vertical discretizations indicates that the principal pressure and effective-stress results are relatively stable. Relative to the base-case grid, the fine-grid differences were 0.25% for maximum pressure, 0.71% for CO₂ saturation, 0.27% for effective stress, and 0.71% for mineral alteration. These results support the use of the 11 × 11 × 10 grid for the principal reservoir-scale pressure and geomechanical assessment, while local near-caprock CO₂ saturation remains more sensitive to vertical resolution.

The simulated reservoir pressure increased from 11.8 to 15.8 MPa, producing a 3.0 MPa reduction in effective vertical stress in the sandstone reservoir, equivalent to approximately 19.3%. The maximum simulated reservoir pressure remained below the adopted caprock fracture-pressure threshold of 19.0 MPa, resulting in a pressure safety margin of 3.2 MPa and a safety ratio of 1.20. Under the assumptions of the synthetic model, the simulated condition therefore remains below the adopted fracture-pressure threshold.

The geochemical alteration modifies the reservoir petrophysical state through the competing effects of mineral dissolution and secondary-mineral precipitation. The resulting changes in porosity and permeability provide a quantitative link between geochemical reactions and fluid-flow evolution. Nevertheless, the effective-stress

reduction in the present model is primarily controlled by pore-pressure increase through the Biot effective-stress relationship.

The first-order Sobol sensitivity analysis identified pressure as the largest individual contributor to the variance of cumulative secondary-mineral precipitation, with a sensitivity contribution of 59%, followed by pH and temperature. This result indicates that pressure is the dominant individual control on the selected geochemical response within the investigated parameter range. Because the Sobol response variable is cumulative secondary-mineral precipitation, the sensitivity results should not be interpreted as a direct ranking of mechanical-failure risk.

Overall, the study provides a reproducible numerical workflow for integrating reactive transport, petrophysical evolution, pressure response, effective stress, and fracture-pressure assessment. The results provide a quantitative basis for evaluating pressure management and long-term CO₂-storage integrity in synthetic saline-aquifer systems. Further work should incorporate heterogeneous reservoir and caprock properties, refined near-caprock grids, site-specific fracture-pressure measurements, and field-scale validation against monitored CO₂-storage projects.

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6. Declarations

6.1 Author contributions

Citra Fitria: Conceptualization, Methodology, Investigation, Data Curation, Visualization, and Writing – Original Draft. Novia Rita: Supervision, Methodology, and Writing – Review & Editing. Ayyi Husbani: Supervision, Validation, and Writing – Review & Editing. All authors have read and approved the final version of the manuscript.

6.2 Funding statement

This research received no specific grant from any funding agency in the public, commercial, or not-for-profit sectors.

6.3 Competing interest

The authors declare that they have no competing interests.

6.4 The use of AI and AI-assisted technology

During the preparation of this manuscript, the authors used ChatGPT (OpenAI) for language editing, formatting support, and improvement of clarity. The authors reviewed and verified all AI-assisted outputs and take full responsibility for the final content of the manuscript.

7. Glossary of terms and symbols

Terms & Symbol	Definition	Unit
CCS	Carbon Capture and Storage	-
CMG-GEM	Computer Modelling Group – Generalized Equation-of-State Model	-
CO ₂	Carbon dioxide	-
ϕ_f	Internal friction angle	degree (°)
SR	Safety ratio (P_f/P_r)	-
Margin	Difference between fracture pressure and reservoir pressure	MPa
A _{i,RSA}	Reactive surface area (RSA)	m ² ·m ⁻³
BHP	Bottom-hole pressure	Mpa
Sobol Index	Global sensitivity index used to quantify parameter influence	-
P	Pore/reservoir pressure	MPa
P ₀	Initial pore pressure	MPa
P _{max}	Maximum simulated reservoir pressure	MPa
P_f	Adopted caprock fracture-pressure threshold	MPa
M	Pressure safety margin; $M = P_f - P_{max}$	MPa
SR	Pressure safety ratio; $SR = P_f/P_{max}$	–
σ	Total stress	MPa
σ'	Effective stress	MPa
$\sigma'_{v,0}$	Initial effective vertical stress	MPa
$\sigma'_{v,max}$	Maximum/final effective vertical stress	MPa
σ'_n	Effective normal stress	MPa
σ_v	Total vertical stress	MPa
$\Delta\sigma'$	Change in effective stress	MPa
ΔP	Change in pore pressure	MPa
α	Biot coefficient	–
E	Young's modulus	MPa or Mpsi
ν	Poisson's ratio	–
C / c	Cohesion	MPa or psi
ϕ	Internal friction angle	degree (°)
τ_f	Shear stress at failure	MPa
k	Permeability	mD
k ₀	Initial permeability	mD
ϕ (porosity)	Reservoir porosity	–
ϕ_0	Initial porosity	–
n	Empirical exponent in the permeability–porosity relationship	–
r _i	Reaction rate of mineral i	mineral amount/time
k _i	Mineral-specific reaction-rate constant	1/time
k _{0,i}	Pre-exponential reaction-rate constant for mineral i	1/time
A _i	Reactive surface area of mineral i	m ² /m ³
Q _i	Ion activity product for mineral i	–
K _{eq,i}	Equilibrium constant for mineral i	–
E _a	Activation energy	J/mol
R	Universal gas constant	J/(mol·K)
T	Absolute temperature	K
TST	Transition State Theory	–
Sg	Gas/CO ₂ saturation	fraction

kr _g	Gas relative permeability	–
kr _{og}	Oil/gas relative permeability term reported in the model	–
Δn Mineral	Change in mineral amount	gmol
n _{initial}	Initial mineral amount	gmol
MA	Mineral alteration metric	%
Sobol index	Variance-based global sensitivity index	–
S _i	First-order Sobol sensitivity index	–
ST	Total-order Sobol sensitivity index	–
Q	Ion activity product / reaction quotient as used in the reaction-rate expression	–
H ₂ CO ₃	Carbonic acid	–
H ⁺	Hydrogen ion	mol/L or activity basis
OH [–]	Hydroxide ion	mol/L or activity basis
HCO ₃ [–]	Bicarbonate ion	mol/L or activity basis
CO ₃ ^{2–}	Carbonate ion	mol/L or activity basis
Ca ²⁺	Calcium ion	mol/L or activity basis
Mg ²⁺	Magnesium ion	mol/L or activity basis
K ⁺	Potassium ion	mol/L or activity basis
Al ³⁺	Aluminium ion	mol/L or activity basis
SiO ₂ (aq)	Dissolved silica species	mol/L or activity basis
P _f	Fracture pressure; equivalent notation to <i>P_f</i>	MPa

8. References

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