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Society of Petroleum Engineers

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Full-Physics CO₂ Storage Modelling in Deep Saline Aquifers: State of the Technology

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Abstract

Deep saline aquifers (DSAs) represent the Earth's largest CO₂ storage resource, constituting approximately 96% of the over 14000 GtCO₂ global aggregated storage resource (OGCI, 2024). Capturing this vast potential for sustainable CO₂ storage in DSAs demands robust modeling frameworks that fully couple advective multiphase flow, reactive transport of CO₂ in the subsurface, capillary and relative permeability hysteresis, CO₂–brine mutual solubility, and poromechanical deformation. However, due to high computational costs and limited research scope, most of the CO₂ storage studies in literature have integrated only a subset of the fully resolved physical, chemical and operational controls that impact field-scale CO₂ storage performance in DSAs, often relying on simplistic assumptions and approximations that may undermine their applicability.

In this study, we present a full-physics simulation framework for CO₂ storage in DSAs integrating a detailed geological model that captures reservoir geometry, seals, and structural features. Our comprehensive framework also includes dynamic multiphase flow characteristics with relative permeability and capillary-pressure hysteresis, and advanced thermodynamics with equation-of-state formulations for supercritical CO₂–brine system. Importantly, we also consider reactive transport modules to capture mineral dissolution, water vaporization, salt precipitation, and mineral trapping in our framework. A 2-way coupled geomechanics for solving injection-induced poroelastic stress-strain relationships and its associated porosity changes, as well as caprock integrity and uplift/subsidence have been also incorporated. Furthermore, near-wellbore processes including brine dry-out and salting-out have been carefully accommodated in our novel framework. Notably, we adopt a high-resolution numerical discretization scheme with local grid refinement feature in order to optimize the accuracy-efficiency trade-off, making our simulation framework a fully resolved, yet applicable solution for field-scale analyses.

The base-case simulation confirmed that sustained CO₂ injection is feasible under the operational bottom hole pressure (BHP) constraints, with three injectors achieving stable target rates over the 30-year injection

period. Post-injection migration was governed by buoyant rise and capillary hysteresis, yielding a plume that remained contained within the primary aquifer and progressively thinned and spread up-dip. After 500 years, CO₂ partitioning was dominated by residual trapping (66%), with smaller contributions from dissolution (11.5%), free phase CO₂ (22%), and negligible mineralization (~0.05%). The model sensitivity to various physical, chemical, and operational controls was investigated. Thin aquifers and low-porosity cases experienced earlier injectivity loss and higher caprock failure potential, while deeper and thicker aquifers sustained higher injection volumes but retained larger proportions of mobile CO₂. Salinity and dip angle strongly influenced plume footprint and trapping partitioning, whereas ambient hydrodynamic flows displaced the plume footprint laterally, shifting the monitoring area of review. Collectively, these results emphasize the importance of full-physics coupling in predictive storage modelling, as simplified approaches risk misrepresenting the balance of trapping mechanisms, plume migration behavior, and long-term geomechanical risks.

Introduction

The 2024 global CCS capacity at approximately 0.05 GtCO₂/yr significantly undercuts the 2050 net-zero demand projections outlined by both the [IPCC \(2022\)](#) and IEA (2021). Additionally, over 80% of currently operational CCS projects feed enhanced oil recovery (CO₂-EOR) processes which historically generate life-cycle CO₂ emissions that exceed their stored CO₂ by a mass factor of two to four ([Godec et al. 2017](#); [Jaramillo et al. 2009](#); [Jiang et al. 2018](#)), alongside inherent scalability constraints related to EOR demand limitations ([Mac Dowell et al., 2017](#); [Núñez-López & Moskal, 2019](#)). Consequently, unlocking the extensive potential for sustainable CO₂ storage in deep saline aquifers (DSAs) is essential for meaningful climate change mitigation ([Benson & Cole, 2008](#); [IPCC, 2022](#)) and necessitates robust numerical modeling frameworks for accurate field-scale prediction of CO₂ storage performance in DSAs ([Sekera & Lichtenberger 2020](#); [Wang et al. 2022](#)).

Current modeling methods in DSAs typically employ substantial simplifications to address computational constraints, resulting in compromised model predictions that tend to increase project risks ([Class et al., 2009](#); [Nordbotten et al., 2005](#)). Analytical and semi-analytical models, though computationally efficient, inherently simplify the physics of complex reservoir heterogeneity and plume dynamics, leading to inaccurate predictions of CO₂ plume migration, as demonstrated in [Figure 1](#) from the benchmark study of [Nordbotten et al. \(2012\)](#). Poorly constrained assumptions in parameterizing multiphase flow - relative permeability functions, and capillary hysteresis - can introduce significant errors in simulated results reducing model validity ([Class et al. 2009](#); [Wang et al. 2022](#)). Similarly, inadequate thermodynamic equation-of-state (EOS) models that neglect critical aspects of CO₂-brine mutual solubility and reactive transport processes can significantly distort accurate prediction of near-wellbore salt precipitation and CO₂ injectivity ([Pruess et al., 2002](#); [Spycher & Pruess, 2005](#)). Ignoring poroelastic coupling and associated geomechanical deformation in CO₂ storage simulations underestimate stress-induced alterations in porosity, permeability, caprock integrity risks, and ground surface displacement, ultimately compromising storage security, operational safety and regulatory compliance ([Mukhopadhyay et al. 2014](#); [Zoback & Gorelick, 2012](#)).

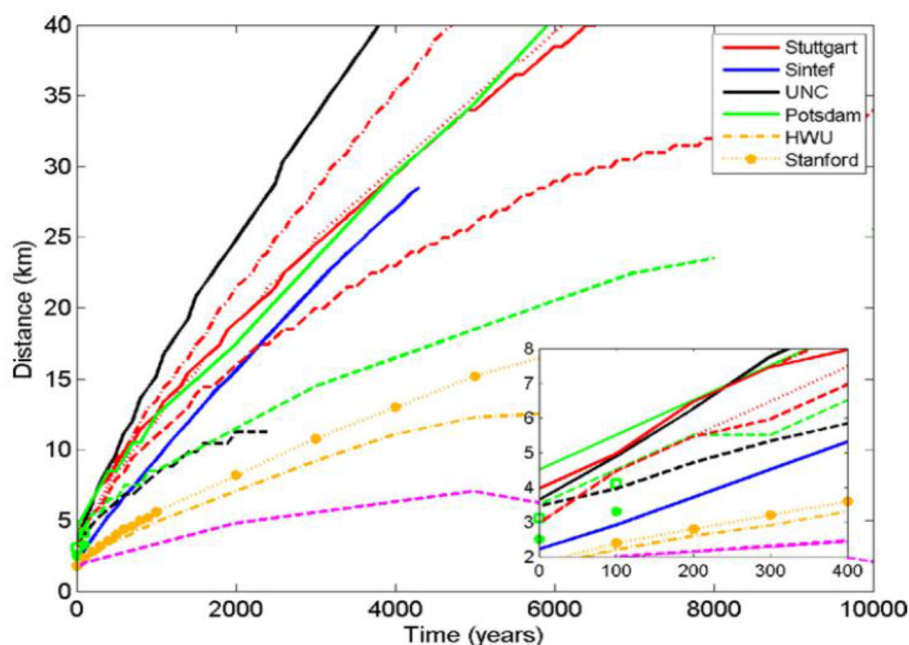


Figure 1—Spread in simulated up-dip extent of plume due to different model simplifications (Nordbotten et al., 2012)

Field-scale modeling studies, such as those conducted at the Sleipner, Gorgon, Snahvit and Illinois Basin Decatur (IBDP) storage projects, highlight the practical consequences of model simplifications. Early CO₂ storage models of Sleipner's Utsira aquifer underestimated the vertical anisotropy of its thin shale layers - resulting in significantly larger CO₂ plume areas than predicted, and higher measurement, monitoring, and verification (MMV) costs (Arts et al., 2004; Ringrose, 2020). The impact of near-wellbore effects resulted in an unplanned well intervention to restore Sleipner's CO₂ injectivity (Hansen et al., 2005). Similarly, fault-compartmentalization and near-wellbore effects were inaccurately predicted for Snohvit's Tubaen aquifer (Eymard et al., 2012; Ringrose & Sxther, 2020) resulting in the suspension of CO₂ injection due to unpredicted rapid pressure increase with no provisions for active pressure management (Simmenes et al., 2013; Buscheck et al., 2016). At the IBDP, initial models excluded important structural uncertainty and heterogeneities, assuming closed boundaries, leading to inaccurate predictions of injection pressures and plume migration pathways (Greenberg et al., 2017; Valluri et al., 2020; Bukar et al., 2025). At the Gorgon CCS project inadequate representation of pressure dissipation and near-wellbore effects has limited injection rates below planned levels with significant cost escalation (IEEFA, 2024).

Addressing these modeling challenges and limitations requires field-scale analogues - full-physics simulation for CO₂ storage in DSAs that integrates all critical controls within a single framework.

Full-Physics Model Framework

A full-physics CO₂ storage model in deep saline aquifers attempts to integrate all the above controls in a single simulation at field-scale. It starts with a high-resolution geological model capturing reservoir extent, thickness, depth, structure, stratigraphy, petrophysics, heterogeneity, anisotropy, faults/fractures and seal integrity. Advective multiphase flow is simulated with hysteretic relative permeability and capillary pressure relationships linked to flow units and capillary rock-types within an ambient hydrodynamic field. Advanced EOS models dynamically compute CO₂-brine thermodynamics and phase behavior (mutual solubility, density, viscosity and enthalpy variations) under evolving pressure-temperature-composition conditions. Reactive transport models resolve both fast aqueous equilibria and slow TST reaction kinetics related to CO₂ dissolution, water vaporization, salt precipitation/ dissolution, and mineral trapping - near-wellbore processes, including brine dry-out and salt- bank formation, are resolved using local fine grids. Two-way

poroelastic coupling updates injection-induced stress, strain, porosity, caprock integrity, and surface uplift/subsidence based on calibrated rock strength, in situ stress regimes and boundary conditions. Realistic operational and regulatory constraints -including well design and patterns, injection strategy and rates, pressure management (BHP limits, brine production), CO₂ supply limits, and MMV requirements - are imposed to ensure practical applicability of the model predictions.

Structure

The modelled reservoir is a 900 km², 100 m thick carbonate aquifer at a depth of 1,500 m, represented with a geometry of 30km × 30km. The structural trap is a four-way dip-closed anticline with a 1° dip at the injection point, and closed boundaries. The primary seal comprises 30 m of anhydrite caprock, overlain by a 10 m thick secondary aquifer and a 10 m thick secondary seal as shown in Figure 2. These overlying units simulate the multi-layer reservoir-seal successions common in many CO₂ storage projects and allow for monitoring and quantification of potential leakage through the primary seal.

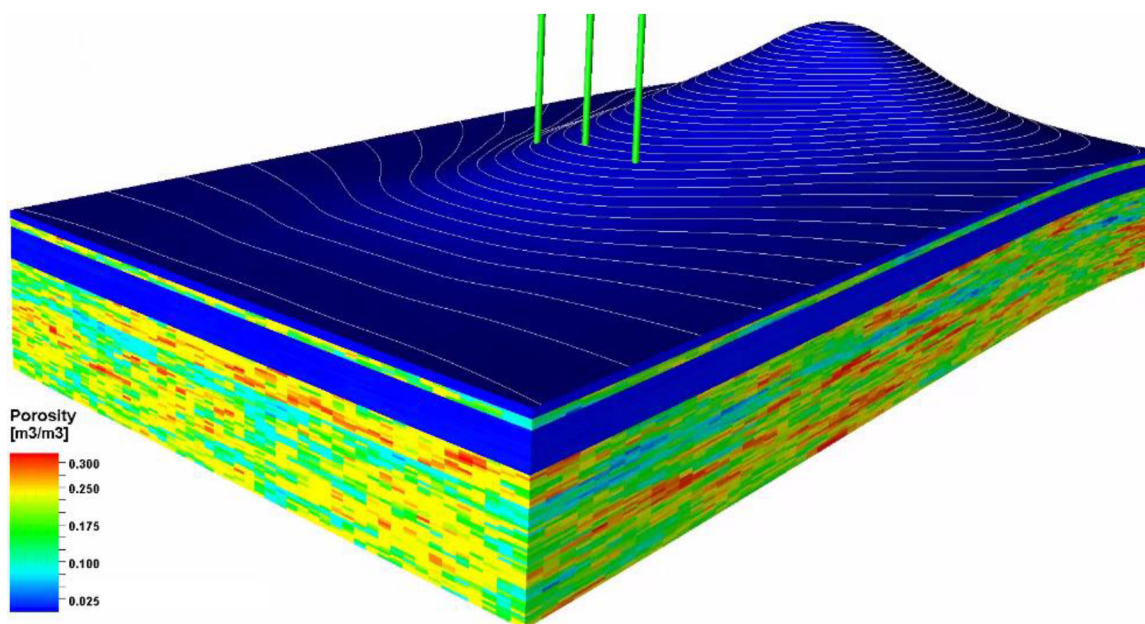


Figure 2—3-dimensional visualization of the base case aquifer porosity model, showing position of injectors, and both primary and secondary aquifers and seals

The base case structural model excludes faults and fractures and assumes a closed pressure boundary at the aquifer limits. The physical grid resolution is 200 × 200 × 2 m, covering a 10 km × 14 km nearfield area, with numerical aquifer extensions beyond the defined model area. This results in the simulation model size of 50 × 70 × 75 = 262,500 grid cells. Local grid refinement is further applied around each injector to improve the resolution of near-wellbore effects.

Petrophysics

The aquifer petrophysical model has a mean porosity of 20% (standard deviation: 4.5%), and a mean permeability of 500 mD (standard deviation defined via heterogeneity). The caprock has mean porosity and permeability of 0.1% and PH) 1×10⁻⁴mD respectively. To capture capillary heterogeneity within the aquifer, a seven-class rock-typing scheme is developed by combining dimensionless proxies for pore diameter (Amaefule et al., 1993) and rock fabric (Lucia, 2007).

$$\text{Gaussian CDF, } \Phi(\mu, \sigma, x) = \frac{1}{2} \left[1 + \operatorname{erf} \left(\frac{x - \mu}{\sigma \sqrt{2}} \right) \right] \quad (1)$$

$$\text{PoreDiameter}, \quad \delta = \Phi \left[a + 0.5 \log_{10}(\phi), 1, \log_{10}(k) \right] \quad (2)$$

$$\text{RockFabric}, \quad m = \Phi \left[b + 5 \log_{10}(\phi + 0.05), 1, \log_{10}(k) \right] \quad (3)$$

with permeability (k) in mD, porosity (ϕ) in fractional units, and constants $a = \log_{10}(k_{\text{mean}}) + 0.3676$, and $b = \log_{10}(k_{\text{mean}}) + 3.5$ scale with the mean aquifer permeability. Table 1 shows the applied RRT cut-offs based on approximate boundaries for carbonate reservoir rock-types.

Table 1—Aquifer rock-typing scheme showing defined cut-offs for each carbonate rock-type (RRT)

RRT	Description Pore	Diameter, δ	Rock Fabric, m
1	Tight	$\delta < 0.014$	-
2	Low Quality	$0.14 \leq \delta < 0.12$	-
3	Mid Quality Unimodal	$0.12 \leq \delta < 0.45$	$m < 0.5$
4	Mid Quality Bimodal	$0.12 \leq \delta < 0.45$	$0.5 \leq m < 0.85$
5	High Quality Bimodal	$\delta \geq 0.45$	$0.5 \leq m < 0.85$
6	High Quality Unimodal	$\delta \geq 0.45$	$m < 0.5$
7	Fractured	-	$m \geq 0.85$

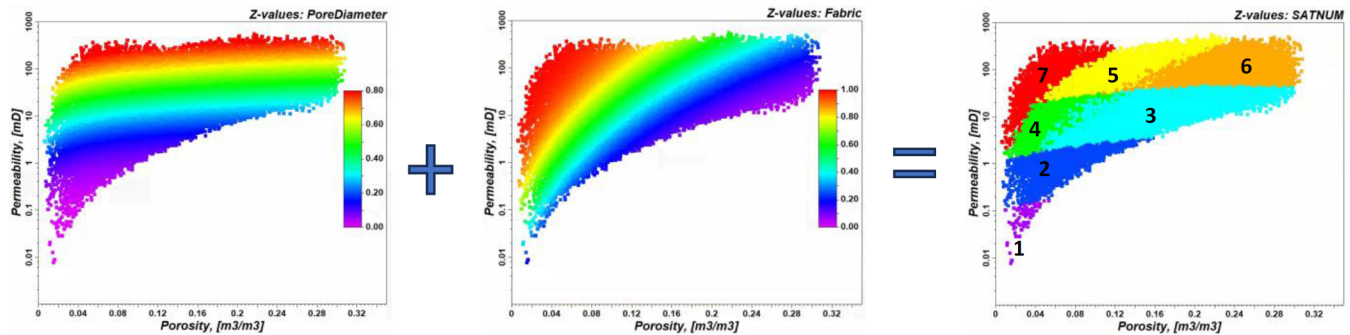


Figure 3—Aquifer rock-typing scheme (right) which combines dimensionless proxies for pore diameter (center) and rock fabric (middle)

Heterogeneity and Anisotropy

The permeability heterogeneity within the aquifer is described using both Dykstra-Parson's coefficient (V_{DP}) (Dykstra & Parsons, 1950) and vertical permeability anisotropy ($V_{kh/kv}$), i.e.,

$$V_{DP} = \frac{K_{50} - K_{84.1}}{K_{50}}; \quad V_{kh/kv} = \log_{10} \left(\frac{k_h}{k_v} \right) \quad (4)$$

where k_{50} is the median permeability, and $k_{84.1}$ the 84.1st percentile of the max-to-min-sorted permeability distribution. The base model parameter values are $V_{DP} = 0.6$, and vertical permeability anisotropy, $V_{kh/kv} = 0.5$.

PVT and EOS

The thermodynamic behavior of CO_2 -brine mixtures is modelled using the hybrid EOS of Spycher et al. (2003) including its extensions to saline and high-temperature conditions (Spycher & Pruess, 2005, 2009). Fugacity coefficients for the CO_2 -rich phase are computed with a modified Redlich-Kwong cubic EOS (Redlich & Kwong 1949), with appropriate mixing rules, and asymmetric binary interaction parameters at higher temperatures, i.e.,

$$P = \frac{RT}{v-b} - \frac{a(T)}{v(v+b)}, \quad (5)$$

where $a(T)$ and b are temperature-dependent attraction and repulsion parameters, and v is the molar volume. Fugacity coefficients (ϕ_i) are calculated from

$$\ln(\phi_i) = \frac{b_i}{b}(Z-1) - \ln(Z-B) - \frac{A}{B} \left(\frac{2 \sum_j y_j a_{ij}}{a} - \frac{b_i}{b} \right) \ln\left(\frac{Z+B}{Z}\right), \quad (6)$$

where Z is the compressibility factor, $A = aP/(RT)^2$, $B = bP/RT$, and y_j are phase mole fractions.

The aqueous phase is treated with activity coefficient formulations, with the pure water component represented using the IAPWS-95 formulation (Wagner & Pruh, 2002). Electrolyte non-idealities are incorporated using Pitzer-type activity models (Pitzer, 1973), where the mean activity coefficient ($\gamma_{\pm}$) reads

$$\ln(\gamma_{\pm}) = -A_{\phi} \frac{\sqrt{I}}{1+b\sqrt{I}} + \sum_{ij} m_j (2B_{ij} + ZC_{ij}). \quad (7)$$

Here I is the ionic strength, A_{ϕ} the Debye-Huckel constant, B_{ij} and C_{ij} are Pitzer parameters, and m_j are molalities.

Salinity effects on brine density, viscosity, and mutual CO_2 –water solubilities are modelled through "salting-out" corrections based on Sechenov coefficients (Sechenov, 1889), which account for ionic-strength suppression of CO_2 solubility.

$$\ln\left(\frac{S_0}{S}\right) = k_s m_s, \quad (8)$$

where S_0 is the solubility in pure water, S is the solubility in saline water, k_s is the Sechenov constant, and m_s is salt molality.

The composite EOS model has been calibrated against experimental data up to 300°C, 600 bar, enabling consistent treatment of coupled phase partitioning, non-ideal mixing, and brine chemistry in reservoir-scale simulations. The fugacity coefficients from the CO_2 –rich phase, and activities of aqueous species, are passed directly to drive CO_2 dissolution, aqueous speciation, and mineral reaction rate laws, ensuring that the reactive transport model is thermodynamically consistent and fully coupled with multiphase flow and compositional phase equilibria at each timestep.

Multi-Phase Flow

Advective multiphase flow is modeled by coupling hysteretic relative permeability and capillary pressure via distinct primary Corey-type drainage/imbibition bounding curves, with Killough (1976) history-aware scanning rules preserving trapped CO_2 while adjusting mobilities as the saturation path evolves. Capillary pressure is expressed using the Brooks-Corey correlation (Skjæveland et al., 2000)

$$p_c(S_w) = \frac{c_w}{\left(\frac{S_w - S_{wr}}{1 - S_{wr}}\right)^{a_w}} + \frac{c_{nw}}{\left(\frac{S_{nw} - S_{nwr}}{1 - S_{nwr}}\right)^{a_{nw}}}, \quad (9)$$

where S , c , and a are saturation, capillary entry pressure and fitting parameters respectively for wetting (w) and non-wetting (nw) phases. Relative permeability is modeled using the generalized Corey form (Corey, 1954), with effective saturations that account for residual trapping, i.e.,

$$k_{rw} = k_{rw}(S_{nwr}) \left[\frac{S_w - S_{wr}}{1 - S_{wr} - S_{nwr}} \right]^{C_w} \quad (10)$$

$$k_{rnw} = k_{rnw}(S_{wr}) \left[\frac{1 - S_w - S_{nwr}}{1 - S_{wr} - S_{nwr}} \right]^{C_{nw}} \quad (11)$$

For each rock-type bounding Corey exponents, end-point saturations, and capillary entry pressures for both drainage and imbibition (Figure 4) are calibrated to experimental datasets (Al-Khdheawi et al. 2017; Edlmann et al. 2018; Chen & DiCarlo 2016; Krevor et al. 2012; Vivek & Kumar 2019), with recent insights on carbonate residual trapping and CO₂ Corey exponents from Wang & Tokunaga (2015) and Masalmeh et al. (2025). The capillary models for each rock-type are applied using J- functions,

$$J = \frac{3.142 P_c}{IFT \cos \theta} \sqrt{\frac{K}{\phi}}, \quad (12)$$

to resolve permeability and porosity-dependent entry pressures at cell-scale. CO₂-brine IFTcos0 is set to 30mN/m.

The ambient hydrodynamic flux for the base case model is set to zero.

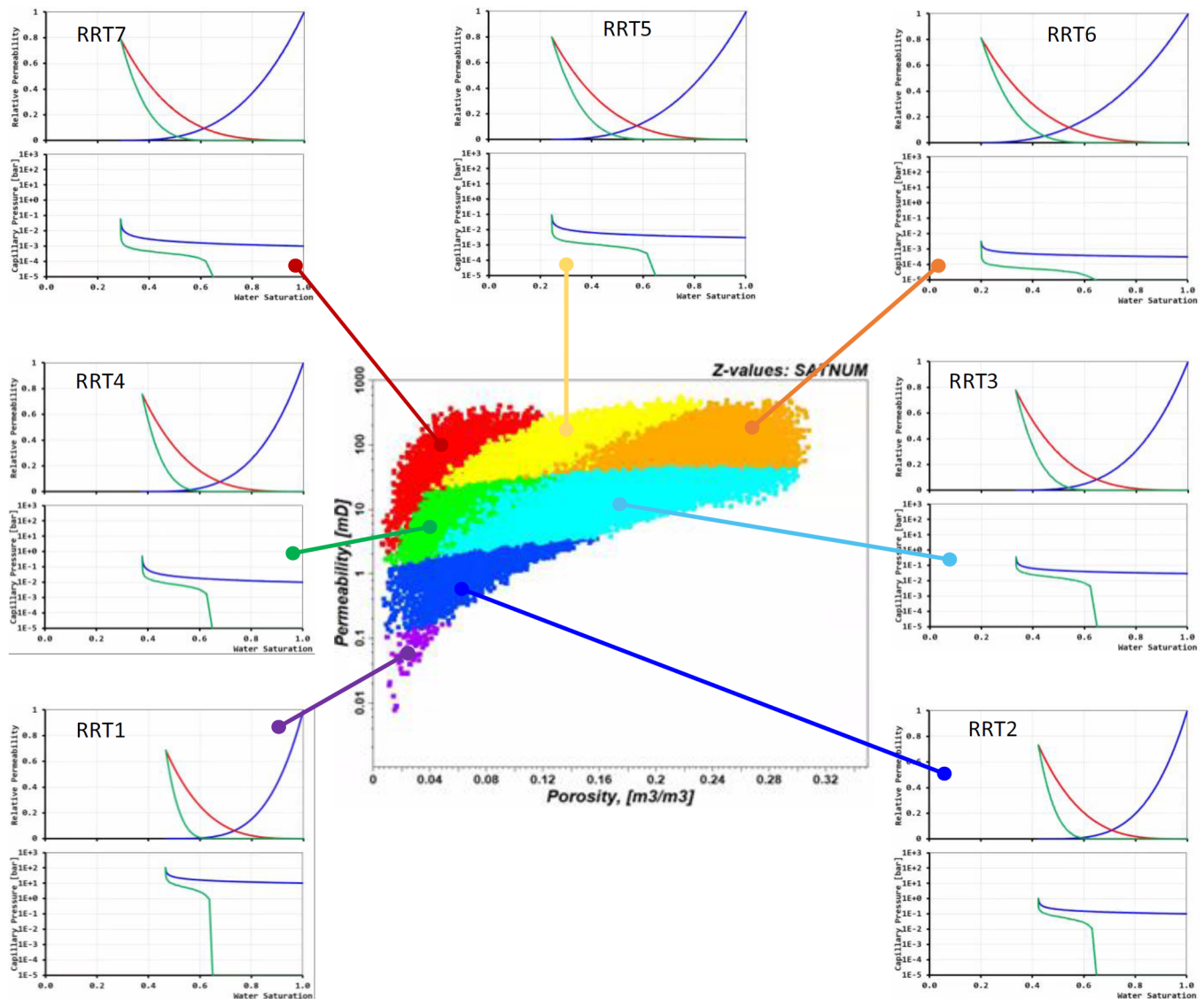


Figure 4—Base case simulation input CO₂ - Brine mobility & capillary hysteresis models matched with aquifer rock-types

Reactive Transport

Reactive transport is fully coupled to multiphase flow by linking CO₂ dissolution, aqueous speciation, and mineral reactions with advective and diffusive transport. Five (5) primary model components (CO₂, H₂O,

NaCl, CaCl₂, CaCO₃) as described in Table 2, are resolved into 13 species: CO₂, H₂O, H⁺, HCO₃⁻, OH⁻, CO₃²⁻, Na⁺, Ca²⁺, Cl⁻, CaCl⁺, NaCl, CaCl₂, and CaCO₃.

Table 2—Standard thermodynamic properties of model components

CO ₂ -Brine Thermodynamic Properties	This Study				
	CO ₂ (Aq./G)	NaCl (Aq./S)	CaCl ₂ (Aq./S)	CaCO ₃ (Aq./S)	H ₂ O (L)
EOS	MRK+IAPWS-15+Fitzer+Sechenov				
	73.82	--	--	--	221.2
Tcrit [T] (K) ci	304.19	--	--	--	647.1
3 Vcrit (m /kmol)	0.094	--	--	--	0.056
Zcrit	0.274367	--	--	--	0.230237
MW (g/mol)	44.01	58.4428	110.986	100.089	18.02
ACF [ra]	0.228	--	--	--	0.343
Parachor	78	--	--	--	52

Four (4) fast equilibrium reactions:



are solved together with three (3) kinetically controlled, transition-state-theory-based mineral dissolution/precipitation reactions:



Under reservoir conditions, brine concentration and salt dry-out induce halite and sinjarite precipitation, while carbonate is treated as calcite. Reaction rates (r) follow the transition-state-theory law, i.e.,

$$r_j = k_j A_j \prod_i a_i^{v_{ij}} \left(1 - \frac{Q_j}{K_j} \right)^{\eta_j} \quad (20)$$

that explicitly includes reactive surface area (A), ion activity (Q) and temperature-dependent equilibrium constants (K) (Lasaga, 1984; Palandri & Kharaka, 2004). Non-ideal aqueous behavior is corrected via a Pitzer-type activity model (Pitzer, 1973) for high-salinity brines. CO₂ dissolution-induced acidification and secondary precipitation alter pore volume and hence porosity, with permeability (k) updated via the Kozeny-Carman relation (Carman, 1956) to reflect mineral volume change, i.e.,

$$k = k_0 \left(\frac{\phi}{\phi_0} \right)^c \left(\frac{1 - \phi_0}{1 - \phi} \right)^2, \quad (21)$$

where the exponent c = 3 for the base case. Phase partitioning employs EOS-derived fugacity coefficients, iteratively updated in each timestep to maintain mass balance within a two-way flow-geochemistry coupling

strategy. Model calibration and validation draw on core-scale studies and established reactive transport behavior in CO₂–brine systems (Duan & Sun, 2003; Mutoru et al., 2010; Espinoza & Santamarina, 2010; Audigane et al., 2007; Mathieson et al., 2011; Khandoozi et al., 2023).

Poroelastic Coupling

The two-way coupled geomechanics model relates the interaction between aquifer pressure, rock strength, and deformation, using carbonate-specific data and empirical models for elastic and strength properties. Porosity-depth corrections (Chen et al, 2020) are applied to capture *in-situ* stress-dependent compressibility. Elastic deformation follows the generalized Hooke's law with porosity and velocity-derived elastic properties (Xu & Payne 2009; Brocher 2005; Gardner et al, 1974; Aki & Richards, 1980; Asef & Farokhrouz, 2017; Khadem et al, 2023). Rock strength properties derive from empirical carbonate models (He et al., 2018) including a graphical solution for Mohr-Coulomb's rock cohesion (Wuerker 1959). In-situ stresses follow from Terzaghi's principle (Terzaghi, 1925) and Hooke's law (Jaeger et al., 2007) assuming a normal stress regime in the base model. These can be stated as

$$\sigma_v = g \int_0^z \rho(z) dz \quad (22)$$

$$\sigma'_h = \frac{\nu}{1-\nu} \sigma'_v - \frac{E}{1-\nu^2} \epsilon_h + \frac{\nu E}{1-\nu^2} \epsilon_H \quad (23)$$

$$\sigma'_H = \frac{\nu}{1-\nu} \sigma'_v - \frac{\nu E}{1-\nu^2} \epsilon_h + \frac{E}{1-\nu^2} \epsilon_H, \quad (24)$$

where E and ν are Young's modulus and Poisson's ratio, effective stress $\sigma' = \sigma - \alpha P_p$, and α is Biot's coefficient.

Injection-induced surface uplift/subsidence due to vertical reservoir expansion (Δh) is based on Geertsma's (1973) model and linked to pore pressure change (ΔP_p) according to

$$\frac{\Delta h}{h} = \alpha \frac{(1-\nu)(1-2\nu)}{(1-\nu)E} \Delta P. \quad (25)$$

The following two failure criteria constrain the poroelastic coupling.

1. Anderson et al, (1973) empirical model which predicts the onset pressure (P_{fp}) for tensile fractures accounting for overburden stress (P_{ob}) and effective pore pressure (αP_p), which can be stated as

$$P_{fp} = \alpha P_p + \frac{2\nu}{(1-\nu)} (P_{ob} - \alpha P_p), \quad (26)$$

and be written in terms of tensile strength σ_T and effective minimum stress σ_3 (compressive stress is positive)

$$\sigma'_3 = (\sigma_3 - \alpha P_p) \leq \sigma_T. \quad (27)$$

2. The Mohr-Coulomb shear failure criterion (Jaeger et al, 2007), i.e.,

$$\tau \geq c + (\sigma_n - \alpha P_p) \tan(\theta), \quad (28)$$

where τ is shear stress, c is cohesion, σ_n is normal stress, and θ is the internal friction angle. The Mohr-Coulomb criterion is applied in its stress tensor form in the simulator, using principal stress limits (Pietruszczak, 2020), i.e.,

$$\sigma^1 - \sigma^3 = (\sigma^1 + \sigma^3) \sin \theta + 2c \cdot \cos \theta, \quad (29)$$

where σ^1 and σ^3 are minimum and maximum principal stresses.

Operational Strategy

The base-case simulation employs a rate- and BHP-controlled continuous CO₂ injection scheme with three (3) deviated injectors (inclination = 70°) spaced 1km apart in a linear pattern, and each injector is operated at a target surface rate of 1.5E3 m³CO₂/day (~1 MtCO₂/year) over a total injection period of 30 years. Injection wells are completed across the bottom third of the aquifer zone with the bottom-hole pressure threshold set to 90% of the fracture pressure (P_{fp}) at the top of perforations, and injection temperature set to match reservoir conditions assuming a preheated CO₂ stream. The pore-pressure threshold of is enforced via automatic rate throttling, to honor caprock integrity constraints. The base model excludes any pressure management or brine producing wells, and injector completion diameter is set to 8.5 inches. The post-injection simulation period spans 500 years for the base case and 200 years for the model sensitivity runs.

Results and Discussion

Base Case Model

The results of the base case simulation show that all three (3) injectors successfully sustained the target injection rates over the 30-year injection period without exceeding the imposed bottom-hole pressure (BHP) constraint, confirming the system's capacity to accommodate stable injection over the timeframe. At the cessation of CO₂ injection, average injectivity had declined by ~60%, while both bottom-hole and average reservoir pressures increased by ~100bar as shown in Figure 5. However, the CO₂ plume remained confined within the primary aquifer, with no leakage detected into the overlying secondary aquifer. The plume geometry was characterized by a compact footprint lefted around the injection cluster, with saturation distributions reflecting the combined effects of viscous drive, early capillary partitioning, and buoyancy displacement.

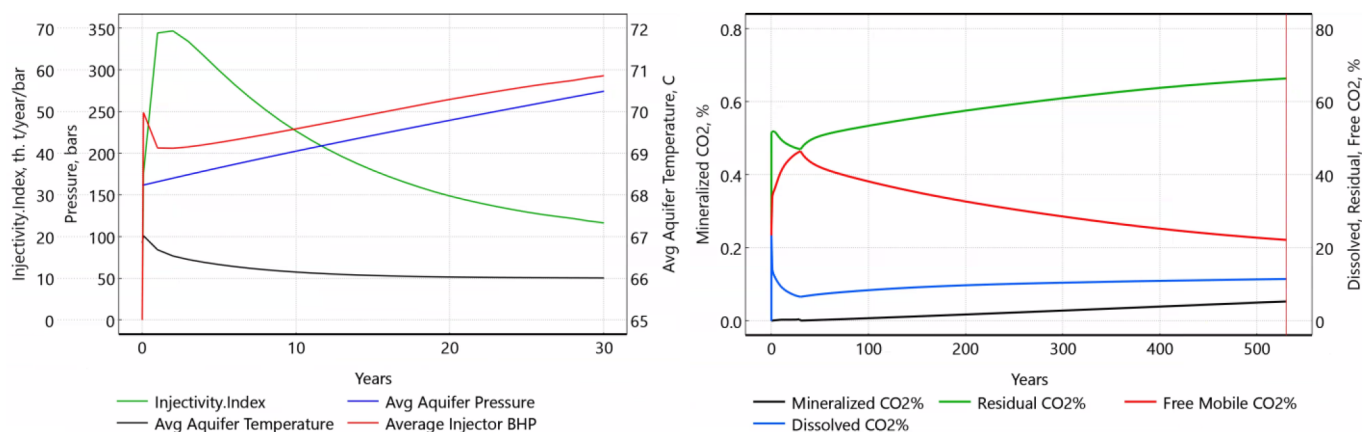


Figure 5—Base case simulated results, showing the evolution of BHP, injectivity, aquifer pressure, and temperature during the injection period (left) and the partitioning of the injected CO₂ by various trapping mechanisms during and post-injection (right)

During the 500-year post-injection monitoring period, the free CO₂ column migrated preferentially up-dip as shown in Figure 6, progressively thinning and spreading laterally toward the structural crest. This migration is governed by buoyancy forces, which promote upward displacement, and counteracted by capillary forces, which enforce entry pressures, and inhibit large-scale remobilization of residually trapped CO₂. The interplay of these forces results in a plume migration distance of approximately 6.5 km (Figure 7), while maintaining vertical containment within the target aquifer.

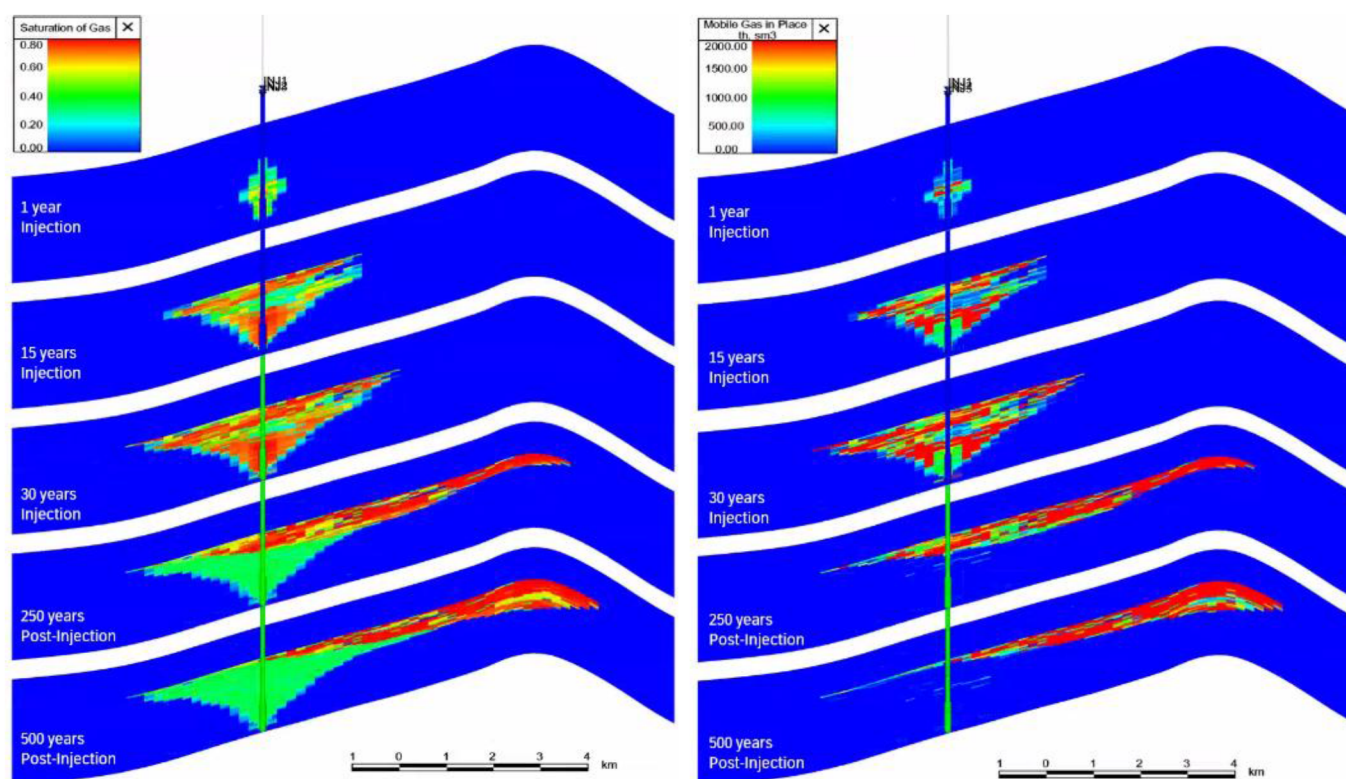


Figure 6—Cross-section of base case model, showing the evolution of sCO₂ phase saturation (left) and the mobile sCO₂ volume in-place (right). The visual difference from L to R highlights the residually immobilized CO₂ trailing end of the plume

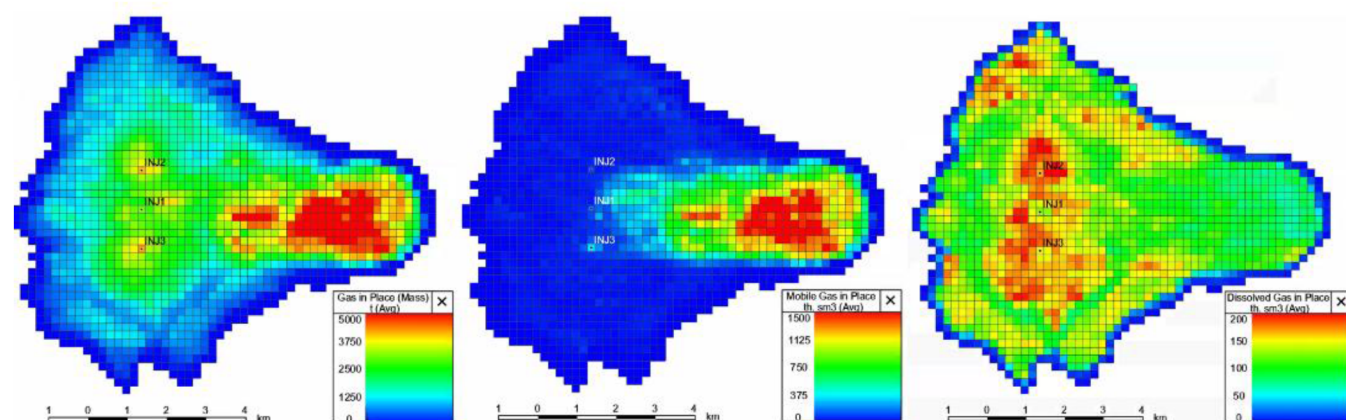


Figure 7—Top view of base case model at the end of simulation, showing the vertically averaged CO₂ mass in-place (left), mobile CO₂ volume in-place (middle), and the dissolved CO₂ volume in-place (right).

By the end of the 530-year simulation period, the trapping partitioning revealed a predominance of residual trapping, accounting for approximately 66.3% of the injected mass, reflecting the role of capillary heterogeneity in restricting CO₂ mobility and fragmenting the plume into disconnected ganglia. The pronounced residual trapping also reflects the impact of permeability and capillary heterogeneity, as well as the 6.5 km plume migrated distance. As shown in Figure 5, solution trapping accounted for 11.5% of the injected mass, consistent with the brine's salinity (150,000 ppm), which suppressed CO₂ solubility relative to lower-salinity systems. Roughly 22.2% of the injected mass persisted in mobile free supercritical CO₂ phase, primarily accumulating beneath the caprock, near the structural crest, where long-term containment is governed by the caprock's capillary and structural barrier. Mineralization contributed only marginally

(~0.05% as CaCO_3), in agreement with the relatively short reaction timescales and modest reactive surface area of the formation (20% average porosity).

Despite the limited bulk mineralization (Figure 5), geochemical reactions provide a notable secondary trapping mechanism within and along the plume margins. During active injection, elevated CO_2 partial pressures drive extensive CO_2 dissolution and brine acidification, developing a region of calcite dissolution within the swept zone, counteracted by calcite precipitation due to evaporative concentration of residual brines. These competing fluxes, depending on residual water saturation, reactive surface area, and high ionic strength can tilt the calcite mass equilibrium between dissolution and precipitation within the plume boundary at the end of injection phase. This process is sustained by continued supply of dissolved CO_2 ($\text{CO}_2(\text{aq})$) diffusing from the free CO_2 phase into the adjacent brine at pore-scale. After injection ceases, the plume pressure relaxes and re-equilibrates with adjacent aquifer, the equilibrium solubility of CO_2 decreases causing partial CO_2 exsolution (Xu et al., 2017) and pH rebound within the plume, which shifts carbonate equilibria toward carbonate and bicarbonate species. The interaction of this CO_2 -rich mixing zone with background alkaline brine during the imbibition produces calcite supersaturation especially around the outer plume boundary, forming a persistent mineral saturation halo that mirrors the end-of-injection plume outline as shown in Figure 8. Beyond this syn-injection plume boundary, the post-injection regime favors net precipitation.

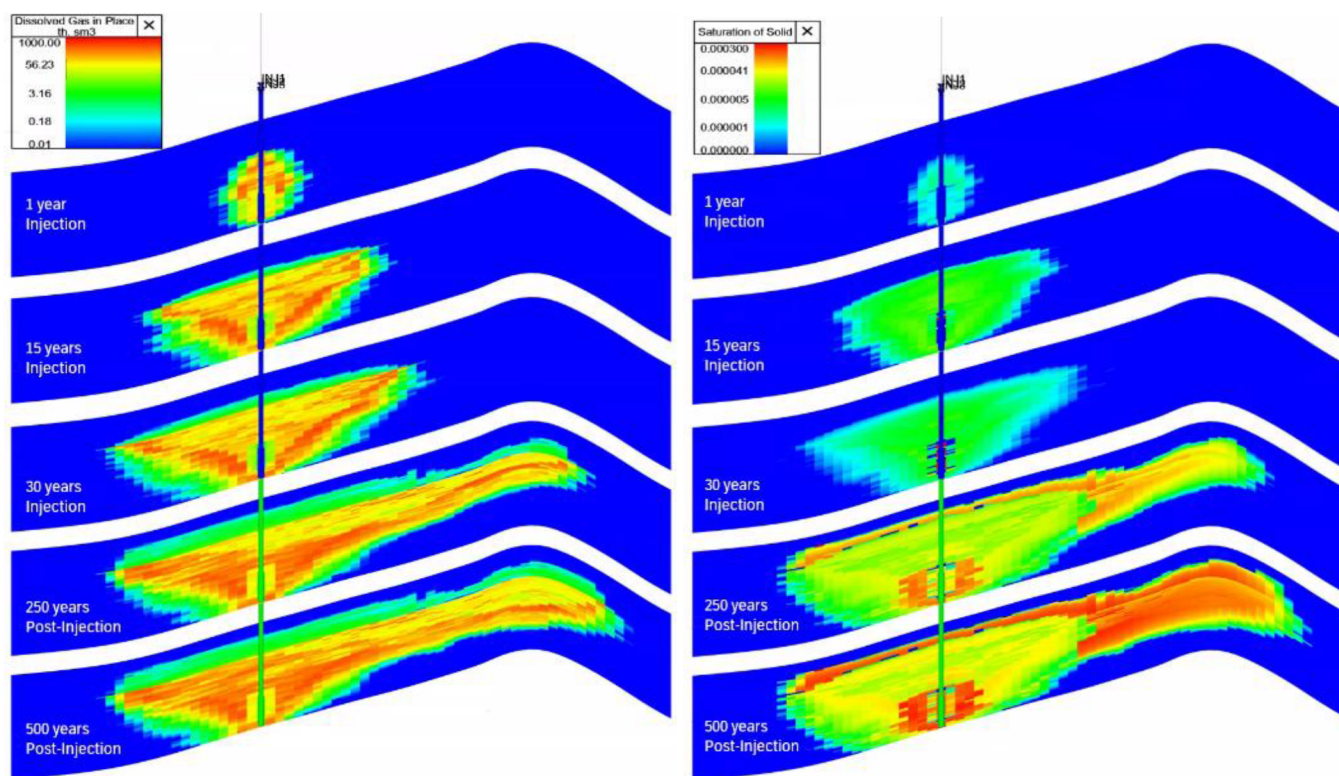


Figure 8—Cross-section of base case model, showing the evolution of dissolved CO_2 in-place (left) and Calcite (solid) saturation(right). The color change around the injectors (left) is due to reduced LGR grid size. The end-of-injection plume boundary halo (right) persists during the post-injection period.

A long-lived, high-density localized brine region remains trapped near each injector (Figure 9) because post-injection CO_2 exsolution is inhibited by a nucleation/capillary barrier and by stable density stratification, and due to the zero ambient hydrodynamic flux. The residual CO_2 dissolution maintains supersaturation, so that the dense carbonated brine decays only diffusively, preserving the near-well density anomaly for centuries.

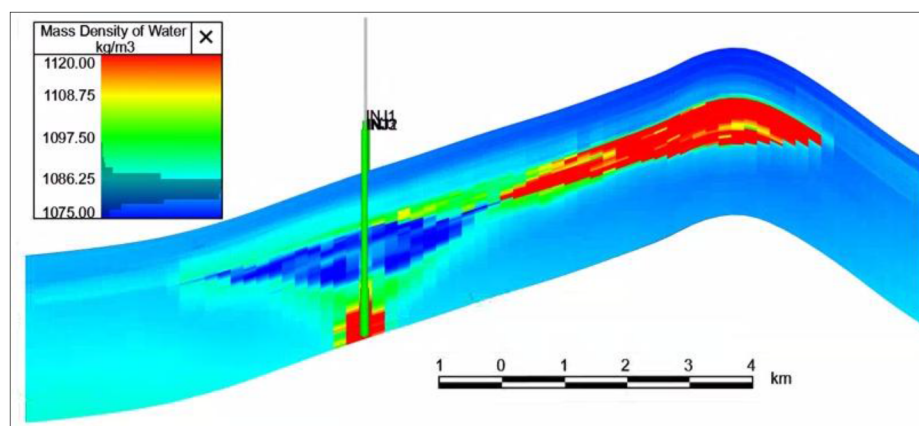


Figure 9—Cross-section of base case model, showing the mass density of brine at the end of simulation. Evaporative supersaturation is visible within the mobile CO₂ phase, and the capillary trapped brine pocket around the injectors.

Geomechanical diagnostics as shown in Figure 11 revealed localized failure events but no large-scale instability. Figure 10 highlights the vertical displacement around the injectors during the early injection period which causes minor roof deformation (uplift) reflecting pressure buildup near the wells. This strain propagates spatially with injection-induced pressure buildup, decaying radially with distance from the injectors. Tensile fractures were observed in the aquifer near the end of injection period as BHP approached the operational threshold. During the post-injection period, localized caprock failure events commenced under increased pressure due to the buoyant CO₂ plume, developing into shear failure zones by the end of the simulation as seen in Figure 11. These caprock failure events remained spatially restricted, suggesting that the stress perturbations subsided as the plume spread thin during its migration, becoming insufficient to propagate continuous rock failure across the caprock.

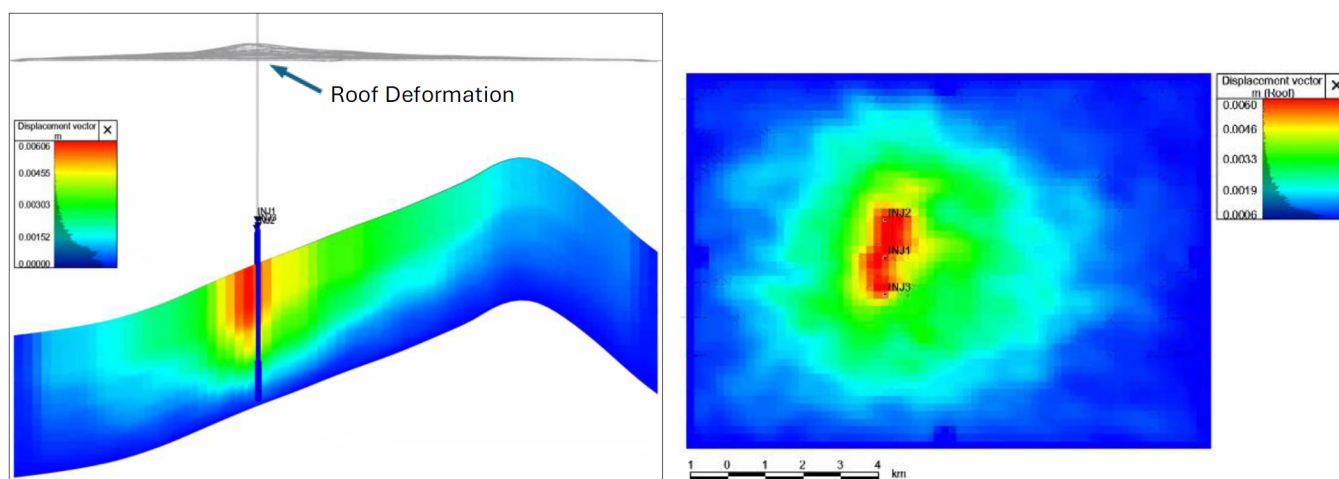


Figure 10—Base case aquifer vertical displacement vector and roof deformation during the early injection stage in cross-section (left) and top view (right).

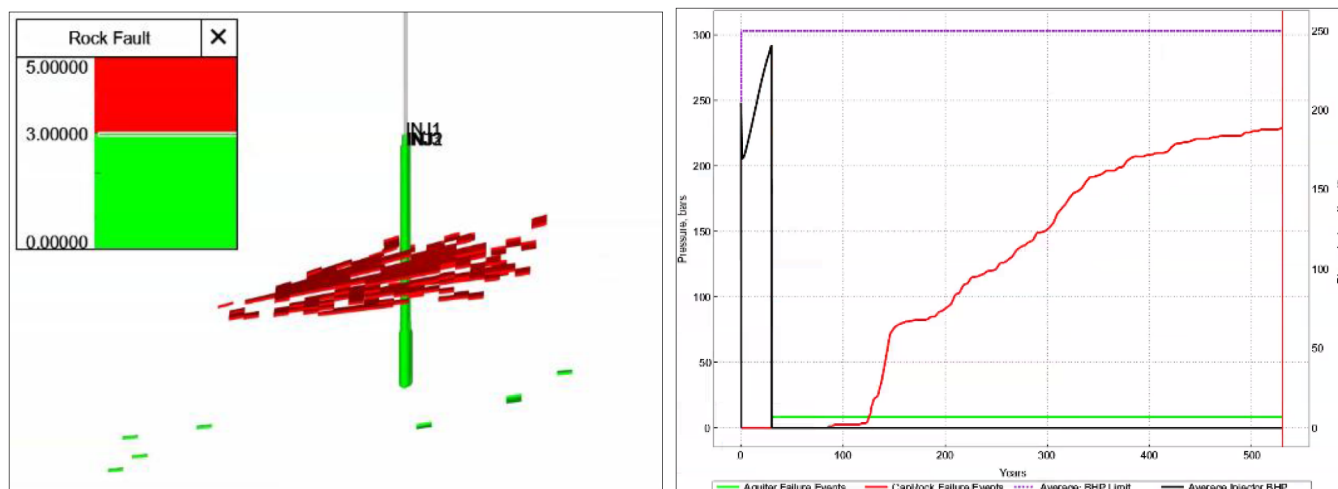


Figure 11—Base case geomechanics coupling, showing tensile (2: green) and shear (5: red) failure events in 3D view (left), and in time-graph with BHP, BHP- limit (right).

Model Sensitivities

The effect of aquifer thickness was investigated by comparing two cases with thicknesses of 50m and 200m, while keeping all other parameters at base case values. In the 50m case, limited thickness led to elevated bottomhole pressures, constrained injection rates, and restricted pressure dissipation. These conditions amplified stress accumulation, triggering a sharp increase in caprock tensile failure events around year 25 as shown in Figure 12, and ultimately forcing premature injection termination. The reduced thickness in the 50m case also forced more lateral plume migration, as shown in Figure 12, increasing the MMV footprint despite a significantly lower cumulative mass of CO₂ injected relative to the 200m case. In contrast, the 200m case sustained target injection rates throughout the injection phase, with a significantly larger vertical capacity, lowering the effective monitoring area and geomechanical failure risk.

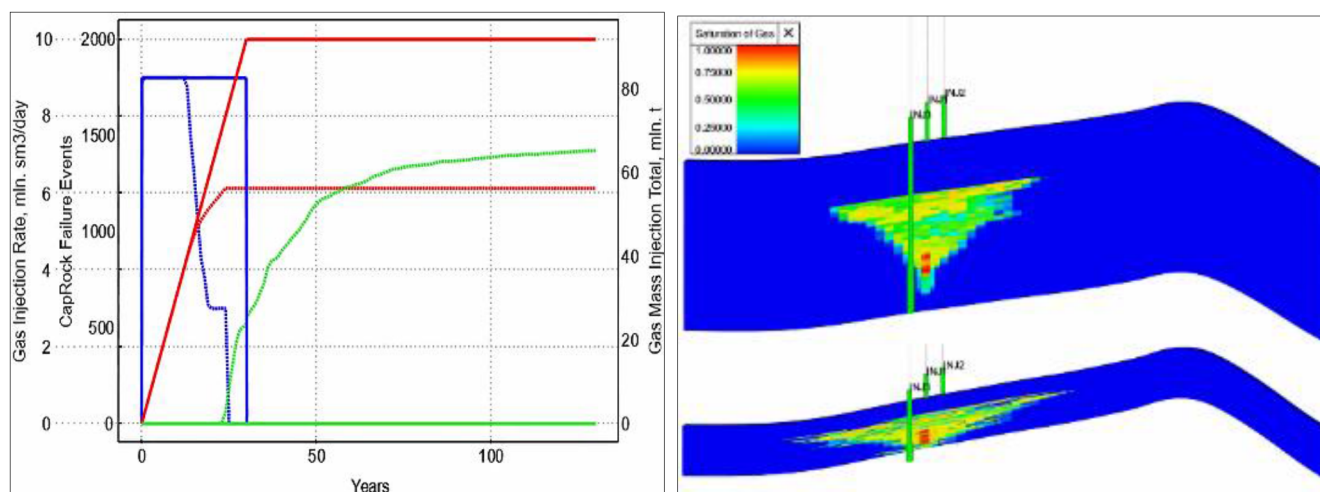


Figure 12—Aquifer thickness sensitivity comparing injection rate (blue), total CO₂ injected (red) and caprock failure events (green) between a 50m (dotted lines) and 200m (solid lines) cases (left); and a cross-section view of CO₂ saturation in both 50m (bottom) and 200m (top) cases at the end of injection period (right).

The influence of CO₂ phase relative permeability Corey exponent (CG) was evaluated using exponents of 2.5 and 5. The increased CO₂ phase mobility at CG = 2.5 increased viscous fingering, which resulted in a larger plume footprint of 48 km², and facilitated improved solubility, mineral, and structural trapping, but reduced the effectiveness of residual capillary trapping as shown in Figure 13. In contrast, the CG = 5 case yielded a more compact plume of 37 km², where reduced phase mobility suppressed solubility and mineral interactions but enhanced residually trapped fraction of injected CO₂.

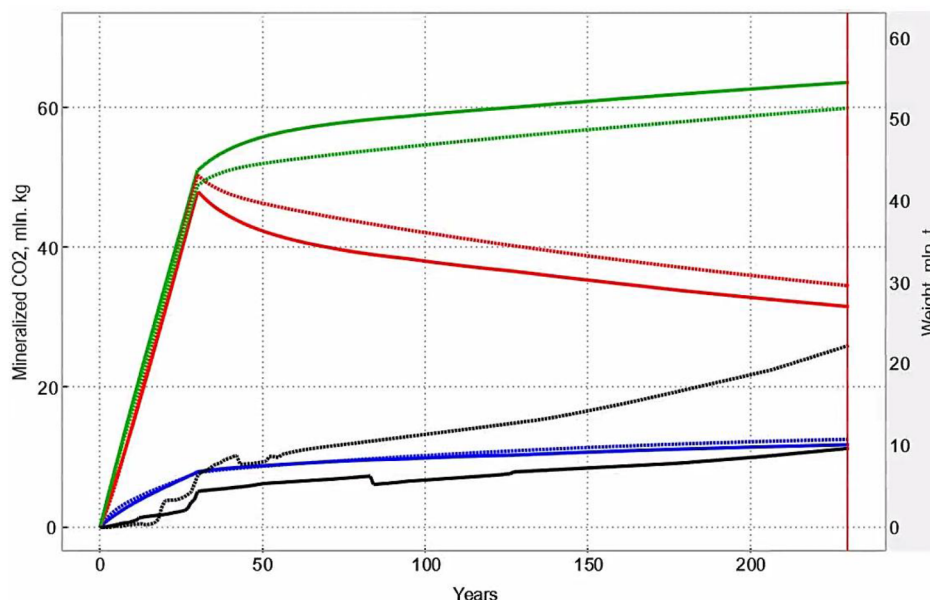


Figure 13—Sensitivity results for CO₂ phase relative permeability comparing Corey exponent of 2.5 (dotted line) and 5 (solid line), showing residual (green), dissolved (blue), free (red) and mineralized (black) CO₂

The impact of background hydrodynamic flow was assessed for two bounding cases representing updip and downdip flow of 0.01 m/day (m³/day/m²). As shown in Figure 14, in the up-dip case (+0.01 m/day), the CO₂ plume exhibited a gradual displacement along the ambient flow direction, with minor asymmetry in plume extent but negligible impact on the overall plume area. In contrast, Figure 14 also illustrates that the downdip case (−0.01 m/day) caused systematic plume advection down- gradient, resulting in a plume shift of approximately 2km relative to the base case. This asymmetric displacement increases monitoring complexity and extends the footprint of pressure perturbation, with implications for MMV planning. While trapping efficiencies were broadly similar between cases, the downdip flow enhanced structural migration risk by biasing plume migration toward the aquifer's structural low, thereby concentrating stress and potentially expanding the area of concern for caprock stability.

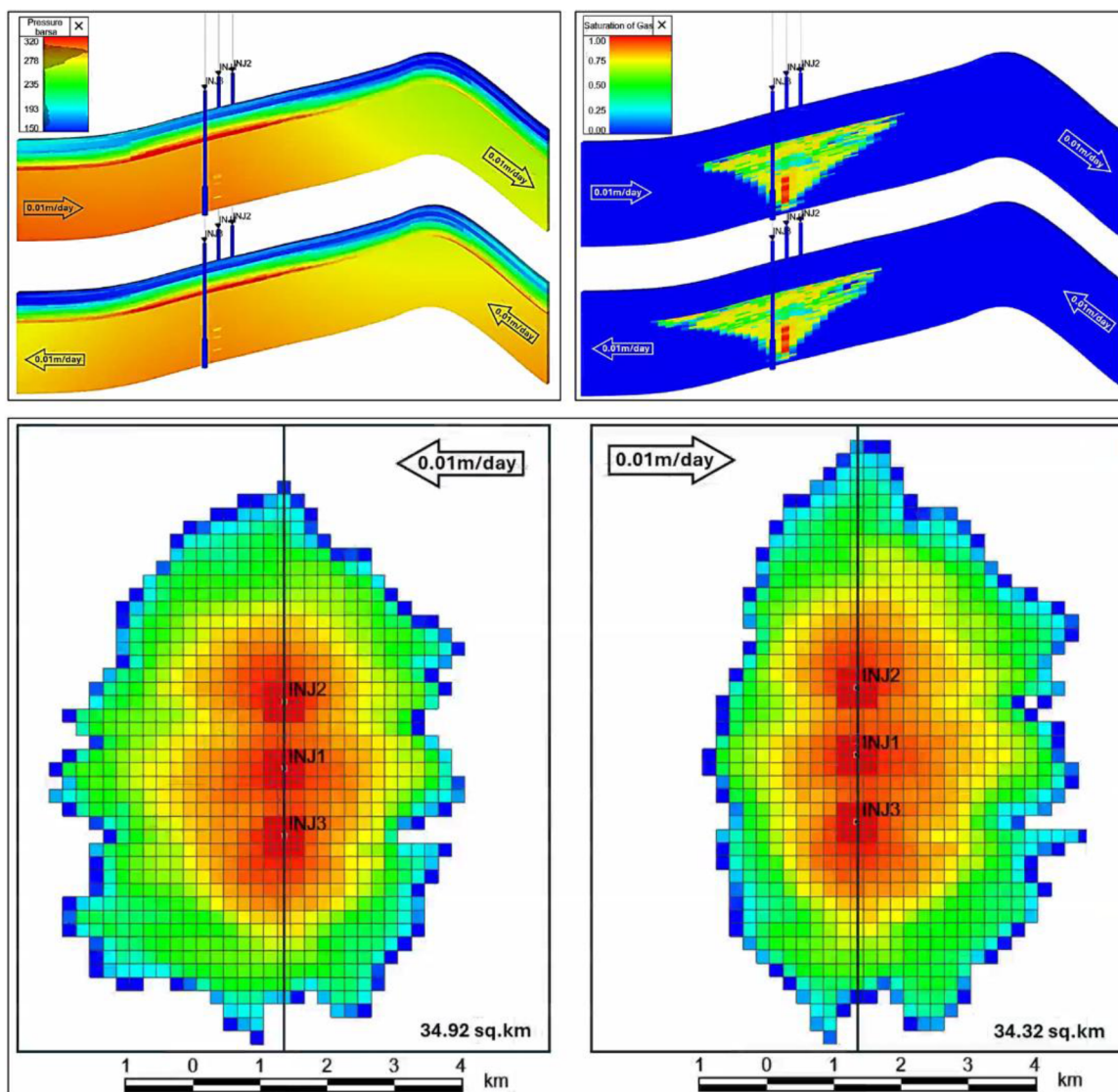


Figure 14—Sensitivity results for ambient hydrodynamic flow in the aquifer comparing flowrates of 0.01 m/day up-dip and 0.01 m/day down-dip, showing end-of-injection pressure distribution (top left), CO₂ Saturation (top right), and plume areas (bottom)

The impact of structural dip was evaluated through two end-member cases of 0.1° and 3° up-dip at the injection point. In the 3° case, as shown in Figure 15, the buoyancy-driven up-dip migration extended the plume to ~ 6.5 km from the injectors, forming an elongated footprint of ~ 40 km². By contrast, the nearly flat 0.1° case produced a more radially symmetric footprint of ~ 47 km², lefted around the injectors. Pressure dissipation was marginally less efficient in the 3° case due to depth-related pressure buildup in the down-dip direction, resulting in elevated BHPs and lower injectivity toward the latter stages of injection as shown in Figure 15. However, the 0.1° case exhibited a sharper post-injection increase in caprock tensile failure events. This behavior reflects the stagnation of the plume around the injectors, where vertical buoyancy loading concentrated stress on the caprock, increasing seal integrity risks relative to the more laterally dispersed plume in the 3° case.

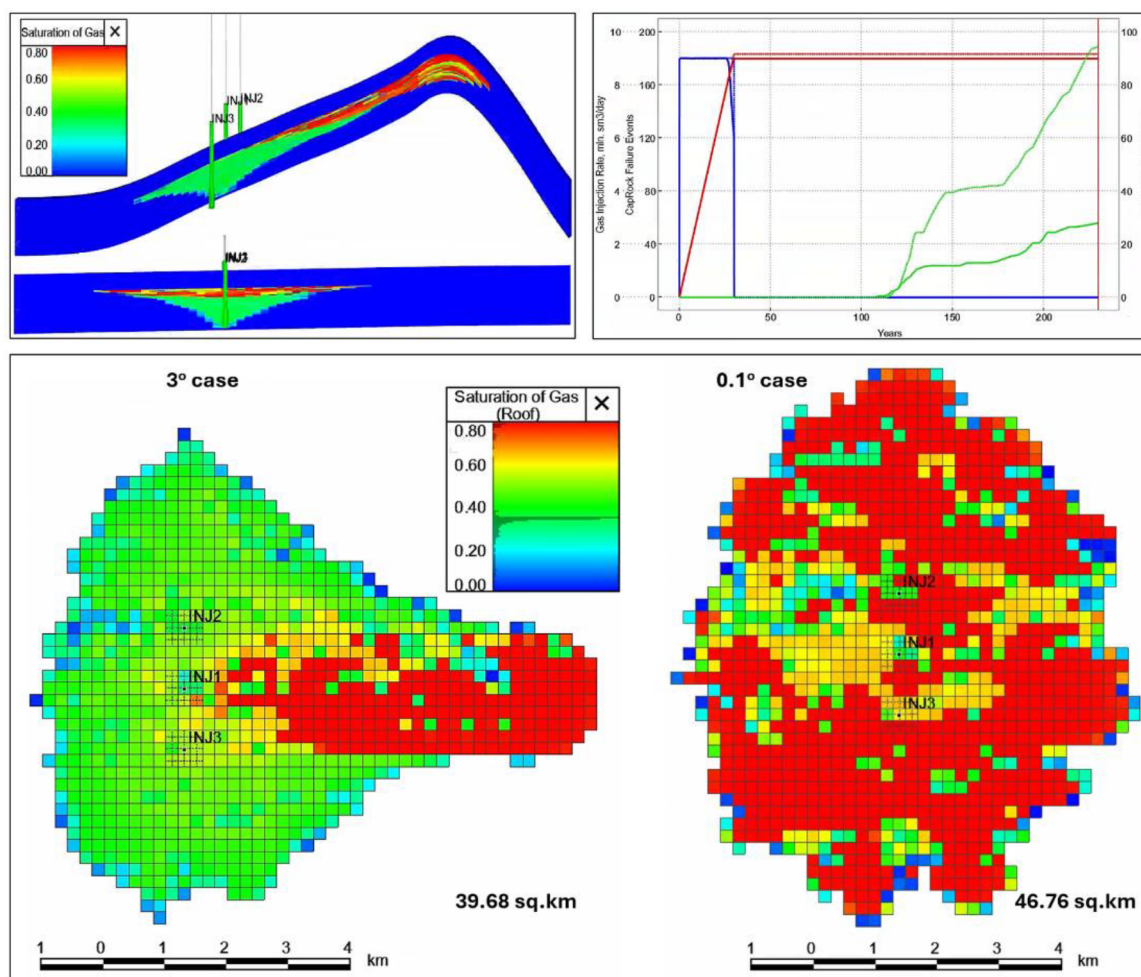


Figure 15—Dip angle sensitivity comparing 0.1° dip and 3° dip, showing end-of-simulation CO₂ Saturation (top left), injection rates (blue) total CO₂ injected (red) caprock failure events (green) (top right), and plume area (bottom)

Two salinity scenarios were evaluated as shown in Figure 16: a low-salinity aquifer (30,000 ppm TDS) and a high-salinity aquifer (300,000 ppm TDS), each composed of a 60:40 NaCl: CaCl₂ mixture by mass. In the high salinity case, the elevated brine density and viscosity produced a steeper hydrostatic gradient, leading to higher initial aquifer pressure and higher BHPs during injection. This pressure buildup, driven by higher brine viscosities, is compounded by enhanced salt precipitation and associated permeability reduction, further limiting injectivity. Additionally, the higher salinity case displayed earlier onset of post-injection caprock instability, consistent with reduced solubility trapping efficiency. As shown in Figure 16, the plume footprint extended to ~50 km² due to increased CO₂ phase mobility arising from stronger viscosity and density contrasts.

By contrast, Figure 17 shows that the low-salinity aquifer exhibited more favorable trapping behavior. Higher CO₂ solubility reduced the mobile phase fraction, delaying caprock failure and lowering the effective area of review. The resulting plume footprint was comparatively smaller (~38 km²), reflecting reduced buoyant drive. The reduced brine viscosity and weaker interfacial tension at lower salinity suppressed capillary immobilization.

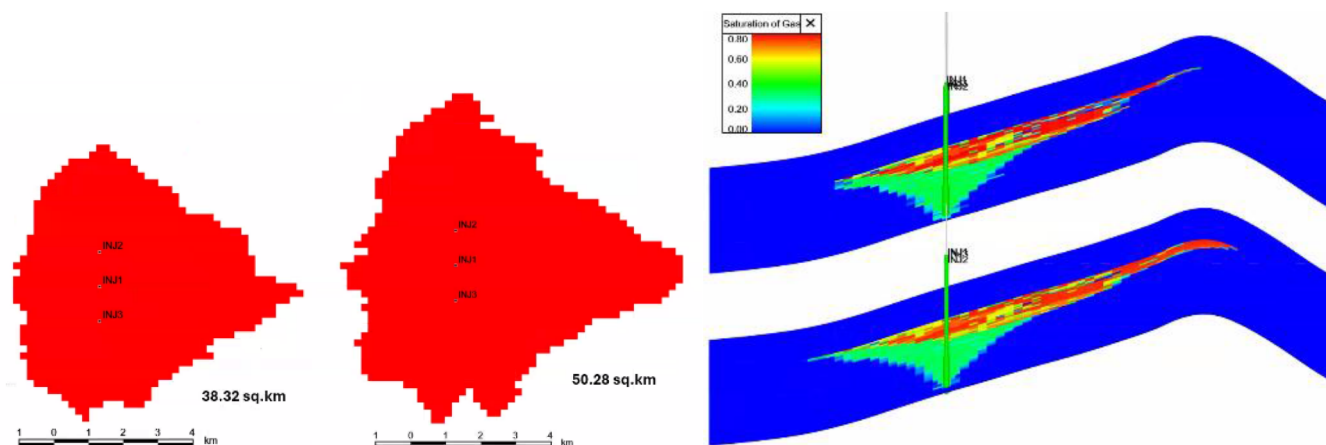


Figure 16—Sensitivity results for aquifer salinity comparing plume area between 30,000 ppm (left), and 300,000 ppm (middle); showing end-of-simulation CO₂ saturation section (right) with 30,000 ppm (top), and 300,000 ppm (bottom)

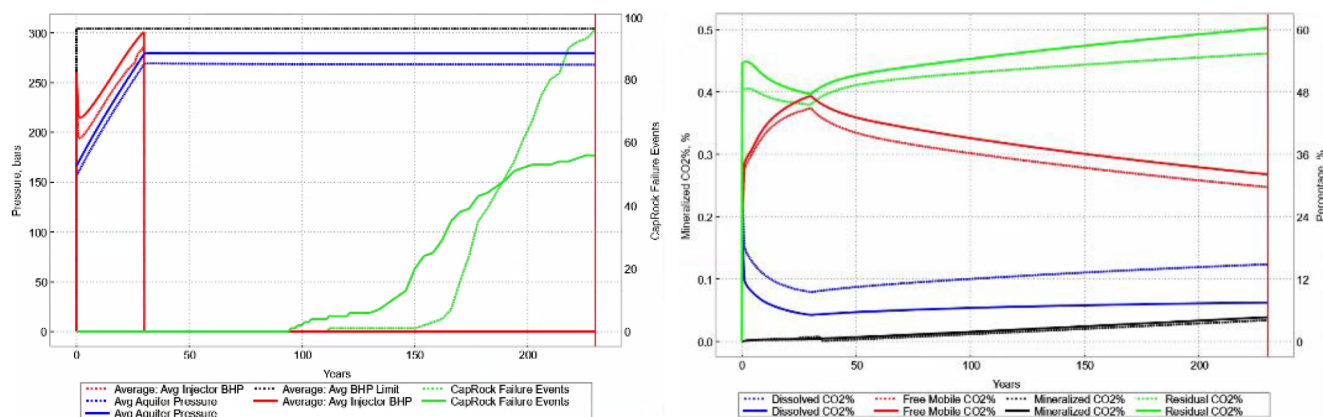


Figure 17—Aquifer salinity sensitivity comparing 30,000 ppm (dotted line) and 300,000 ppm (solid line) showing average injector BHP, aquifer pressure and caprock failure events (left); and trapping partitioning (right)

Two cases of average porosity (10% and 30%) were simulated with other controls kept constant to assess the effect of pore volume. The results are presented in Figure 18. In the low-porosity case (10%), the reduced pore volume (1,587 vs. 4,470 Mrm³ in the 30% case) and lower total compressibility led to elevated bottomhole and average reservoir pressures, which limited pressure dissipation and constrained injection rates. This resulted in premature termination of injection prior to the 30-year design period and ~30% lower cumulative CO₂ storage compared to the high porosity case (30%). The associated stress buildup triggered caprock failure events near the end of the injection phase, whereas the high-porosity case exhibited stable pressure evolution and no mechanical failures.

Trapping efficiencies further differentiated between the two cases. When normalized against the respective cumulative CO₂ injected, the high porosity case favored solubility trapping, whereas the low porosity case relied more on residual trapping, with both cases retaining a comparable fraction of injected CO₂ in the free phase. Despite its smaller pore volume occupancy (82 Mrm³ vs. 142 Mrm³ in the 30% case), representing 5.17% and 3.17% of aquifer pore volume within the modeled area, respectively, the low porosity case produced a disproportionately wider plume footprint (46 km² vs. 30 km² in the 30% case) as shown in Figure 19. This indicates that, at similar permeabilities, lower porosity aquifers may paradoxically yield broader plume migration despite reduced storage capacity, amplifying MMV challenges and mechanical failure risks.

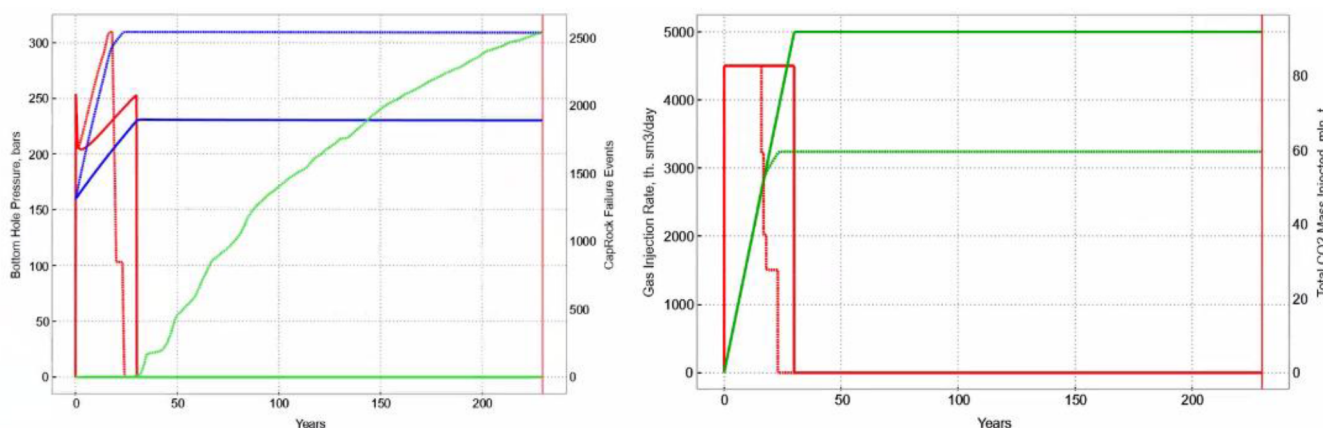


Figure 18—Average aquifer porosity sensitivity comparing 10% (dotted line) and 30% (solid line) showing average injector BHP, aquifer pressure and caprock failure events (left); and trapping partitioning (middle), and injection performance (right)

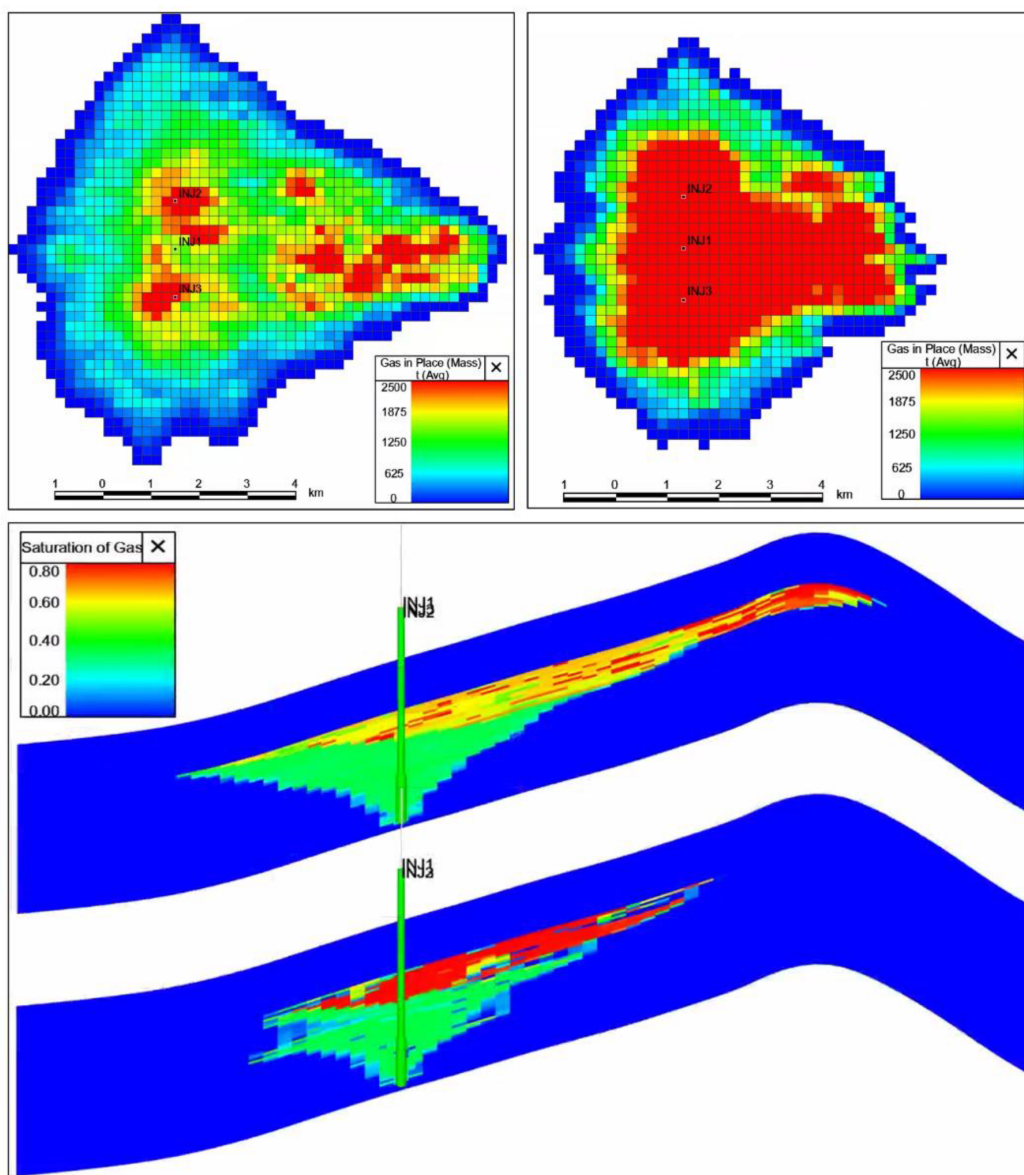


Figure 19—Average aquifer porosity sensitivity comparing plume area between 10% (top left) and 30% (top right) at end-of-simulation; and CO₂ saturation section (right) with 10% (top), and 30% (bottom)

Two aquifer depth cases (800m and 2500m) were simulated. As shown in Figure 20, in the shallower depth (800 m) case, lower fracture pressures and reduced BHP thresholds constrained injectivity, which combined with lower CO₂ density limited cumulative mass of CO₂ stored by ~27% compared to the deeper (2500 m) case. Figure 20 also compares the normalized trapping partitioning showing enhanced retention at shallow depths, with more than double the solubility of the deeper case. Also, capillary immobilization increased by ~10% compared to the deep aquifer. By contrast, the 2500m case retained significantly more free-phase CO₂, consistent with, increased salinity, reduced CO₂ solubility and stronger density-viscosity contrasts. Despite the higher storage capacity, BHPs at 2500m depth were more than double those at 800m, underscoring depth dependent hydrostatic gradients, and fracture pressures.

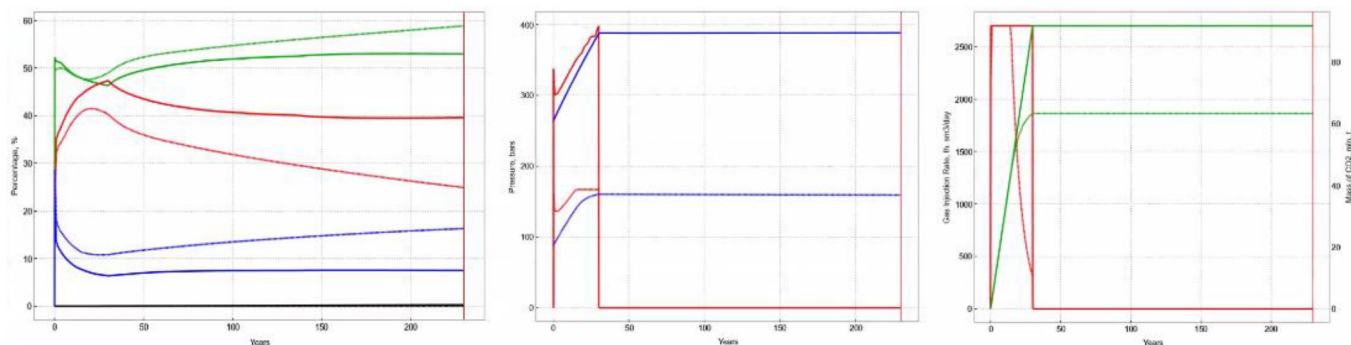


Figure 20—Average aquifer depth sensitivity comparing between 800m (dotted lines) and 2500m (solid lines), showing trapped partitioning (left), pressure profiles (middle) and injection performance (right)

At the end of the 200-year post-injection phase, as shown in Figure 21, the shallow case exhibited a thinner and more widespread free CO₂ column, whereas the deeper case maintained a thicker, more localized column. This contrast in plume morphologies can be explained using the relative density gradients of supercritical CO₂ and formation brine with depth. While brine density increases gradually with depth due to pressure and salinity, its compressibility is low, producing only a modest gradient (typically ~1.0 g/cm³ near surface to ~1.15-1.2 g/cm³ at 2500-3000 m). By contrast, supercritical CO₂ exhibits a markedly steeper density increase with pressure in the 8-25 MPa range, rising from ~200-300 kg/m³ at 800 m to ~700-800 kg/m³ at 2500m. This difference in compressibility produces a sharp reduction in the CO₂-brine density contrast with depth, and significantly higher buoyancy forces at 800m tends to flatten and spread out the plume.

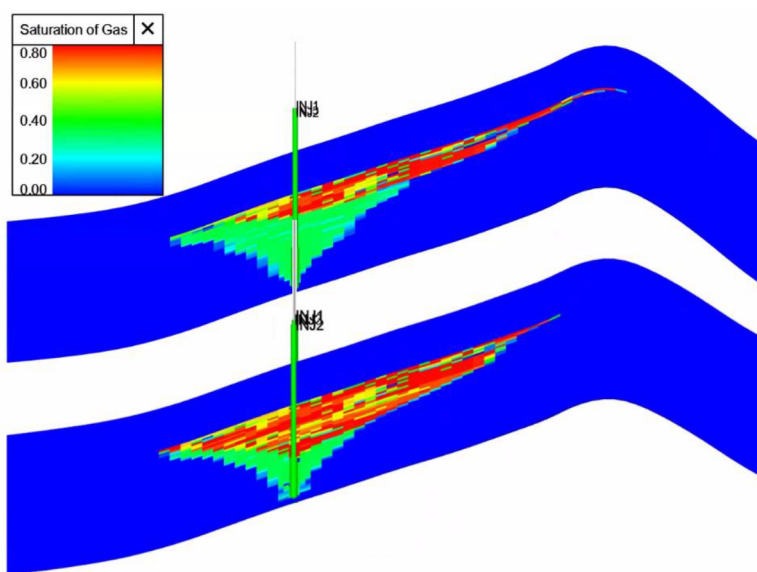


Figure 21—Average aquifer depth sensitivity comparing between 800m (top) and 2500m (bottom), showing end-of-simulation CO₂ saturation section

Conclusion

This study presented a fully coupled reservoir simulation framework integrating multiphase flow, hysteretic relative permeability and capillarity, thermodynamic phase equilibria, reactive transport, and poroelastic geomechanical feedbacks. The model resolves the interplay between injection performance, trapping processes, geochemical alteration, and mechanical stability under realistic operational and geological constraints.

The base case simulation at 1500 m depth (20% porosity, 100 mD permeability, 150,000 ppm salinity) demonstrated that target injection rates could be sustained over a 30-year period without exceeding bottom-hole pressure thresholds, confirming operational feasibility within design limits. At shut-in, the plume was contained within the primary aquifer with no leakage into the overlying secondary units. Over 500 years of post-injection evolution, the plume migrated up-dip, thinning and spreading laterally, while trapping partitioning showed residual immobilization as the dominant long-term mechanism (66.3%), followed by dissolution (11.5%), mobile free CO₂ (22.2%), and negligible mineralization (~0.05%). Reactive transport revealed a persistent calcite precipitation rim along the end-of-injection plume boundary, sustained by residual CO₂ diffusion, pH rebound, and localized supersaturation during post-injection equilibration. Geomechanical coupling identified localized tensile and shear failures in the aquifer and caprock, but no evidence of system-wide integrity loss.

A series of sensitivity analyses highlighted how reservoir properties and boundary conditions govern injection performance and long-term storage security. Thinner aquifers (50m) amplified pressure buildup and induced early tensile failure, while thicker aquifers (200m) enhanced injectivity and stability. Variations in Corey exponents for CO₂ phase altered plume mobility and trapping partitioning, with higher mobility enhancing solubility but reducing capillary trapping. Ambient hydrodynamic flow displaced the plume centroid by over a kilometer, extending the monitoring footprint. Dip angle strongly modulated plume geometry, with shallow dips concentrating buoyancy beneath injectors and steeper dips favoring lateral migration. Salinity was shown to control both hydrostatic gradients and solubility trapping, with higher salinity increasing plume mobility and failure risk. Porosity directly influenced storage capacity and plume footprint, where low porosity reduced cumulative storage but paradoxically yielded broader plume spread. Depth exerted a dual control, with shallow reservoirs favoring solubility trapping and lateral plume

migration, while deeper reservoirs supported larger injection volumes but retained more mobile CO₂ and exhibited higher BHPs.

Overall, the results emphasize that storage security and performance are emergent properties of coupled physical, chemical, and mechanical processes, rather than single-parameter functions. The full-physics modeling framework captures these interactions explicitly, enabling robust assessment of containment risks and enabling the formulation of optimal operational strategies for CO₂ storage projects.

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