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Analytical Vertical Equilibrium Model Accounting for Fines Migration and CO₂-Water Partial Miscibility

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Summary

The injection of humid (or wet) CO₂ into geological aquifers offers a practical means of mitigating near-wellbore impairment caused by connate-water evaporation and the consequent formation damage induced by salt-precipitation in the dry zone. This study aims to develop a novel analytical model for this process. We extend the traditional Vertical Equilibrium (VE) formulation for immiscible displacement of brine by CO₂ in layer-cake reservoirs to incorporate partial brine- CO₂ miscibility, and formation damage due to fines migration and salt precipitation in the dry zone. The depth-averaging of the quasi-2D VE model yields explicit expressions for upscaled phase permeabilities and effective capillary pressure. The resulting 1D model allows for an exact self-similar solution, which provides explicit expressions for determining sweep efficiency and injectivity decline. The analysis of the model reveals the emergence of two distinct displacement fronts—a CO₂ dissolution-displacement front (advanced front) and a full-evaporation front (receded front)—which delineate the two-phase flow region. The explicit analytical expressions derived enable rapid multivariate sensitivity studies on how CO₂ humidity, reservoir heterogeneity, viscosity ratio and formation damage parameters influence overall sweep efficiency and well injectivity.

Introduction

Effective storage of CO₂ in deep saline aquifers relies on the accurate prediction of both storage capacity and well injectivity. However, uncertainties in geological structure, rock–fluid properties, and operational conditions require extensive sensitivity analyses, making full-physics numerical simulation computationally demanding. The development of analytical models provides an efficient alternative, delivering rapid solutions, accelerating inversion and history-matching workflows, and offering clear insight into how reservoir and fluid properties influence the key storage metrics (MacMinn et al. 2010, 2011, Bedrikovetsky 2013). One such promising approach is the development of reduced-order models based on the condition of Vertical Equilibrium (VE). The introduction of VE pseudo-functions reduces the dimensionality of flow

problems in (r,z,t) or (x,z,t) domains to simplified models in (r,t) or (x,t) (Alamara et al. 2023, Guo et al. 2014; Nilsen et al. 2011; Anderson et al. 2015). VE models have therefore become widely used for early-stage screening and conceptual evaluation of CO₂ storage projects in depleted gas fields and aquifers (Alamara et al. 2025)

Traditional VE formulations assume immiscible displacement (Bruining 2021), with associated pseudo-functions derived under the assumption that CO₂ and brine remain compositionally fixed during flow (Yortsos 1995; Zapata & Lake 1981; Coats et al. 1971) for either gravity-dominated or capillary-dominated regimes. Several extensions of the immiscible VE models have been extensively developed to accommodate several flow assumptions and reservoir structures, as reflected by the enormous body of literature on the subject (Eldoy et al. 1985; Zapata and Lake 1981; Coats et al. 1971; Sorbie et al 1994; Yortsos 1992, 1995; Bedrikovetsky 2013; Alamara et al. 2023). These formulations capture layered heterogeneity and vertical segregation but neglect several processes known to exert a strong influence on injectivity and plume evolution. In particular, humidity effects, partial miscibility, salt precipitation, and fines migration can substantially alter phase mobilities, transition-zone behaviour, overall sweep efficiency and long-term storage.

The humidity of the injected CO₂ plays a central role in near-wellbore behaviour. When dry or under-saturated CO₂ enters the aquifer, water evaporates into the CO₂ across capillary-controlled menisci, leading to salt supersaturation and pore-scale salt precipitation (Russell and Bedrikovetsky 2024; Smith et al, 2025). This mechanism is widely recognised as a major contributor to injectivity decline in CO₂ storage projects (Zhang et al. 2025). At the same time, the detachment, transport, and straining of reservoir fines further reduces permeability in the gas-occupied region, amplifying injectivity losses while modifying fractional-flow behaviour (Ge et al. 2022; Wang et al. 2022; Muneer et al. 2022; Othman et al. 2019; Wang et al. 2022). These effects intensify when the capillary transition zone becomes large relative to reservoir thickness, or when rock heterogeneity exhibits strong variation of permeability with depth, $k(z)$. The variations in $k(z)$ interact with capillary forces to shape the nature of fractional flow curves and front stability (Raza et al. 2015; Rasheed et al. 2020; Raza et al. 2019). Another source of complexity is partial miscibility, that is, the dissolution of CO₂ into brine and the vaporization of water into CO₂, resulting in spatial variations in composition and mobility that cannot be captured by classical immiscible VE formulations. The coupled influence of miscibility, humidity, salt precipitation, fines migration, and heterogeneity creates displacement dynamics far more intricate than those represented by classical immiscible VE models. This gap is particularly important because these processes jointly govern injectivity decline, transition-zone structure, and sweep efficiency which are necessary performance metrics for CO₂ storage in geological formations.

Motivated by these limitations, this study develops a novel analytical VE model for radial CO₂-brine displacement in layer-cake aquifers that accounts for: (i) partial CO₂-brine miscibility; (ii) brine evaporation and associated salt precipitation in the dry zone; and (iii) formation damage due to fines migration. By applying depth-averaging on the quasi-2D VE system, we obtain explicit formulae for upscaled phase permeabilities and effective capillary pressure. The resulting 1D hyperbolic conservation law admits an exact self-similar solution that captures the emergence of two displacement fronts: a CO₂ dissolution-displacement front (advanced front) and an evaporation front (receded front), which bound the two-phase flow region. The explicit expressions for saturations, concentration of CO₂, sweep efficiency, and injectivity enable rapid multivariate sensitivity studies, providing clear insight into how CO₂ humidity, reservoir heterogeneity, viscosity ratio, and fines-migration parameters jointly control injectivity and storage performance.

This paper is organized into six main sections. The study first reviews the physical mechanisms governing CO₂-brine displacement and outlines their relevance to the modelling frameworks presented here. The study then introduces the model assumption, followed by a description of the vertical averaging procedure and the

resulting pseudo-functions. The subsequent part of this study develops the self-similar analytical solution to the 1D governing equations, including the derivation of pressure diffusivity equation in the undisturbed region and expressions for pressure and total mobility. A comprehensive sensitivity analysis is performed to examine the influence of key reservoir parameters on flow dynamics and injectivity. The paper concludes with a summary of the main findings and key implications of the study.

2D (r,z)-model for partly miscible displacement in layer-cake reservoir under fines migration

This part of the paper first outlines the key assumptions underpinning the vertical-equilibrium (VE) model, followed by a description of the upscaling procedure and the derivation of the averaged pseudo-functions for saturation, overall concentration, and fractional flow.

Assumptions and formulation of 2D model

In the two-phase region, the gaseous and aqueous phases contain both CO₂ and brine components. We assume that Amagat's law of additive volumes applies during the mixing of these components, and that the individual densities of brine and CO₂ are the same in each phase. This assumption allows the use of volumetric concentrations to represent the components, which can be expressed as:

$$\rho_g = c_w \rho^W + (1 - c_w) \rho^G, \rho_w = c_g \rho^G + (1 - c_g) \rho^W \quad (1)$$

where ρ^G and ρ^W denote the densities of the pure components, while ρ_w and ρ_g are phase densities. It is assumed that the phases have attained equilibrium states hence, c_w and c_g are constant, representing the fraction of brine vaporised into gas and the fraction of gas dissolved in brine, respectively, at a fixed temperature and pressure as shown in Fig. 1.

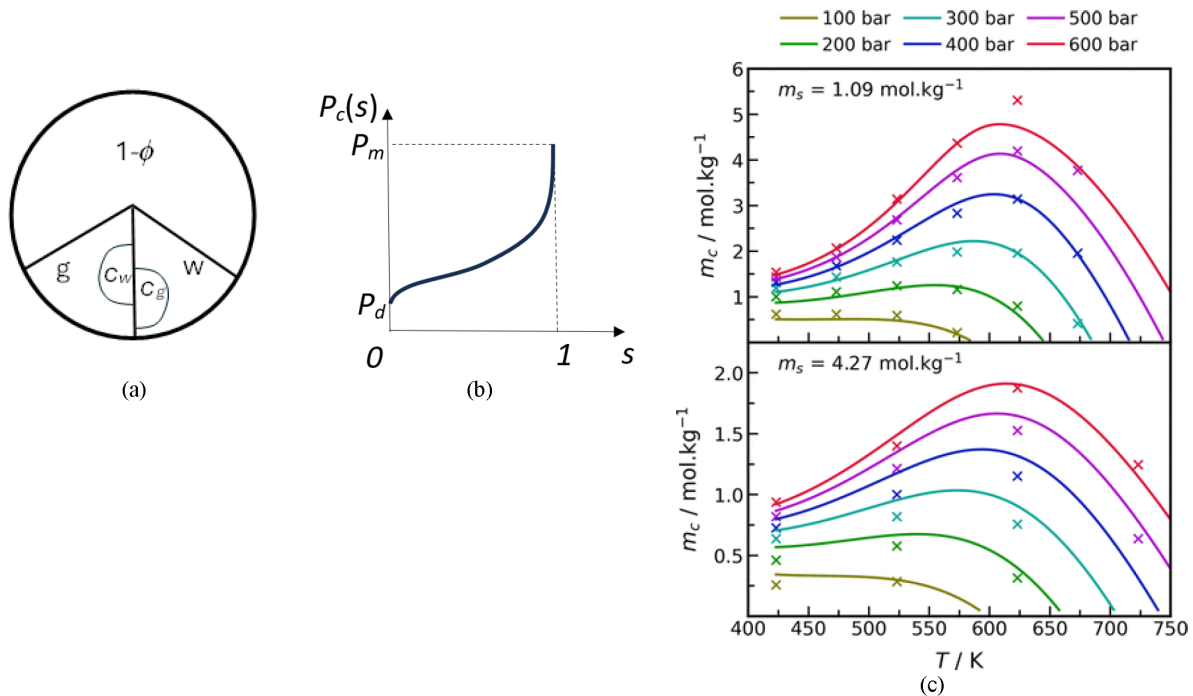


Figure 1—Details of a two-phase system in porous media: (a) volumetric composition of brine and CO₂ components within each phase; (b) Illustration of CO₂ solubility in NaCl solution at elevated temperatures ($T > 423$ K) by Coelho et al. 2025, comparing predictions from the eCPA EoS (continuous curve) with experimental measurements (Takenouchi 1965) (marked points) for varying pressures and salinities of 1.09 and 4.27 mol.kg⁻¹.

The flux of gas and volumetric concentration of CO₂ are given as

$$\tilde{u}_{gr} = (1 - c_w)u_{gr} + c_g u_{wr}, \quad \tilde{C}_g = (1 - c_w)s + c_g(1 - s) \quad (2)$$

The pressure distribution in each phase varies only due to the weight of the fluid column above a given datum. This assumption of hydrostatic pressure in each phase is expressed as

$$\frac{\partial p_g}{\partial z} = -\rho_g g, \quad \frac{\partial p_w}{\partial z} = -\rho_w g \quad (3)$$

The rock is assumed to remain water-wet throughout the displacement process, hence

$$p_c(s) = p_g - p_w \quad (4)$$

and the capillary pressure is defined in terms of the dimensionless Leverett function $J(s)$ as

$$p_c(s) = \frac{\sigma \cos \theta}{\sqrt{k(z)/\phi}} J(s) \quad (5)$$

In this study, we examine the impact of formation damage caused by fines migration and salt precipitation. At the reservoir scale, it is assumed that the processes of fines detachment, migration, and straining occur almost instantaneously relative to the time required for one pore volume injection (PVI) of CO₂. The capillary force acting to detach fines from the rock surface is significantly stronger than the attaching electrostatic force. Consequently, all detachable fines are released by the advancing gas-brine menisci as it passes through a pore (illustrated in Fig. 2). Therefore, the concentration of attached fines within the rock depends on saturation and is described by the maximum retention function (MRF) (Russell et al. 2025; Nguyen et al. 2022). Laboratory experiments indicate that the MRF can be effectively approximated by a power-law relationship (Nguyen et al. 2022).

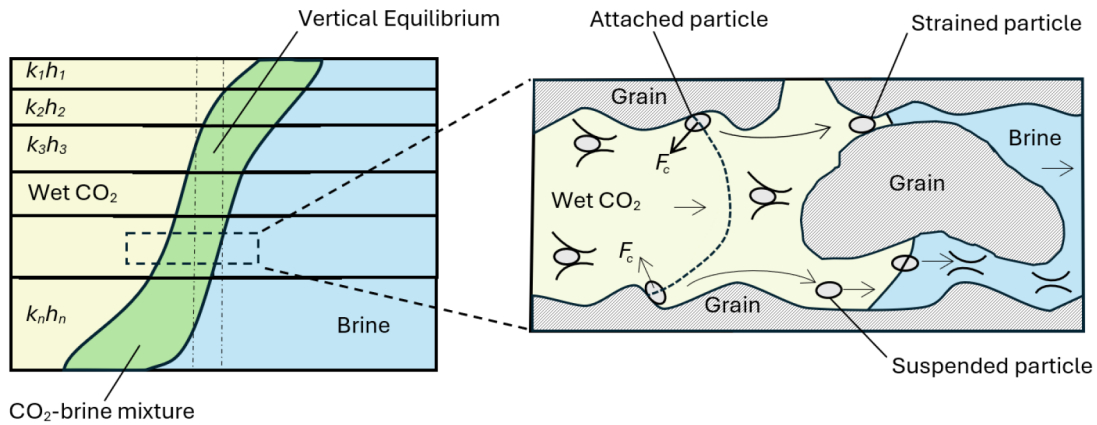


Figure 2—Schematic illustrating two-phase flow processes accounting for fines detachment, transport, and straining in pore constrictions

$$\sigma_{cr}(s) = \sigma_l(s)^B \quad (6)$$

The initial concentration of attached fines, denoted as σ_l and the power law exponent for straining, B , characterize the retention behaviour. The concentration of strained fines, $\Delta\sigma_{cr}$, at a given saturation s is defined as the difference between the initial and current attached concentrations:

$$\Delta\sigma_{cr} = \sigma_{cr}(1) - \sigma_{cr}(s), \quad (7)$$

In the undisturbed zone containing reservoir brine, the hydrostatic pressure distribution follows Eq. (3). Within this region, both the reservoir brine and the rock matrix are considered to have low compressibility, that is,

$$\phi(p)\rho_w(p) = \phi_0\rho_{w0}\exp\left[-\frac{p-p_0}{c_t}\right] \quad (8)$$

Where the index "0" refers to initial conditions, and c_t represents the total compressibility for the rock and fluid (Dake 1983).

The dry zone containing CO₂ is considered to have a hydrostatic pressure distribution with depth as well. In this zone, pressure changes are assumed negligible, so the gas density remains constant. Salt precipitation occurs in the dry-out zone following the displacement of brine by gas, potentially causing significant injectivity decline (Zhang et al. 2025). It is assumed that salt precipitates instantaneously once all brine has evaporated into the gaseous phase. This dry zone forms behind the receded front and is occupied by the displacing CO₂.

Recent advances in the thermodynamic description of CO₂-water and CO₂-brine systems have significantly improved the prediction of phase behaviour under storage conditions. For example, new Cubic-Plus-Association (CPA) and Electrolyte Cubic-Plus-Association (eCPA) equations of state that account for CO₂-H₂O cross-association have been shown to reproduce CO₂ solubility, phase diagrams, and density variations over a wide range of pressures, temperatures, and salinities using Gibbs ensemble Monte Carlo (GEMC) simulations (Coelho et al. 2025). The PVT properties for the CO₂-brine system discussed in this study adopt the correlations proposed by Coelho et al. 2025 which incorporates data from Bando et al. 2003, Lui et al. 2021, Takenouchi 1965 and Yan et al. 2011. The correlation proposed in this recent study capture the subtle increase or decrease in aqueous-phase density associated with CO₂ dissolution, and remain accurate even under geothermal and deep-sequestration conditions.

Fig. 3 presents a schematic of brine displacement by CO₂. Ahead of the displacement front, no CO₂ is present. Hence;

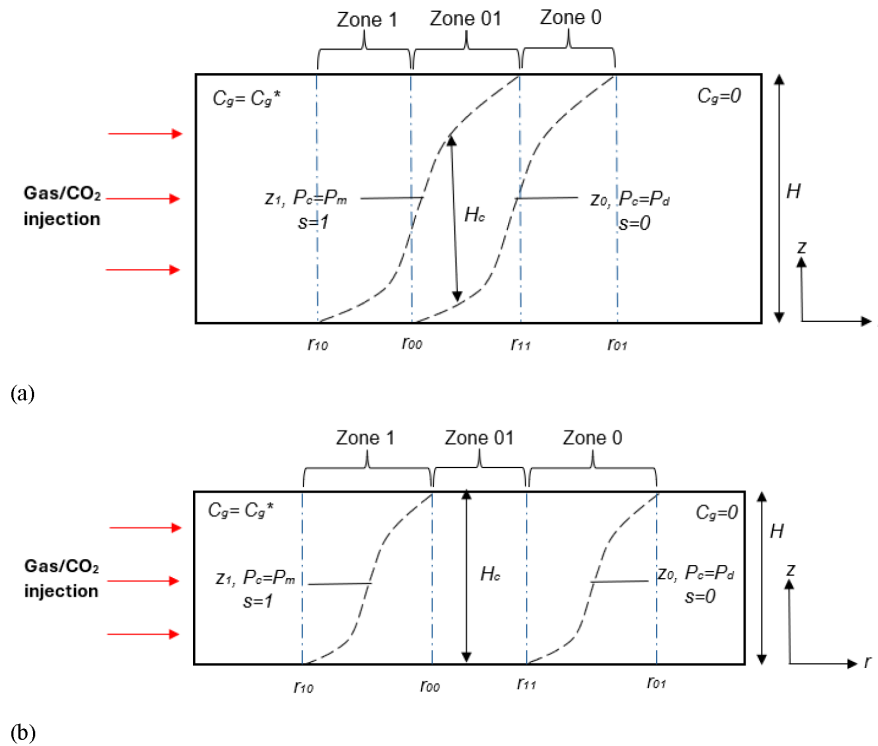


Figure 3—Illustration of water displacement by CO₂ incorporating water evaporation and CO₂ dissolution: (a) displacement in a thick reservoir; (b) displacement in a thin reservoir.

$$z < z_0(r, t), s = 0, c_g = 0 \quad (9)$$

Behind the receded or rear front of complete evaporation, no brine remains.

$$z > z_1(r, t), s = 1, \quad c_g = c_g^* \quad (10)$$

Therefore, the gas saturation is $s=0$ ahead of the displacement front and $s=1$ behind the rear front.

The Darcy's law for gas phase velocity is modified to account for the formation damage due to both fines migration and salt precipitation by introducing two resistance term into the effective permeability of gas. The phase velocities are expressed as

$$u_{gr} = - \frac{k(z)k_{rg}(s)}{\mu_g[1 + \beta_s \Delta \sigma_{cr}(s) + \beta_a a]} \frac{\partial p_g}{\partial r}, \quad u_{wr} = - \frac{k(z)k_{rw}(s)}{\mu_w} \frac{\partial p_w}{\partial r} \quad (11)$$

where β_s, β_a are the formation damage coefficient due to fines migration and salt precipitation, respectively, and a is the concentration of precipitant behind the dry-out zone front.

Derivation of the averaged pseudo-functions for saturation, overall concentration and fractional flow

Here, the upscaling approach for determining pseudo-functions for saturation, overall concentration and fractional flow is highlighted. In this study, the average gas saturation across the reservoir depth is determined by the expression

$$S(r, t) = \frac{1}{H} \int_0^H s(r, z, t) dz \quad (12)$$

Zone 0 represents the vertical section of the flow domain corresponding to the transition region above the brine phase. Zone 01 and Zone 1 represent the vertical sections corresponding to the transition region between the gas and brine phases, and the transition region above the gas phase, respectively as shown in Fig. 3, i.e.,

$$\text{, i.e.,} \quad 0: r_{11} < r < r_{01}, \quad 01: r_{00} < r < r_{11}, \quad 1: r_{10} < r < r_{00} \quad (13)$$

The fractional flow of the gaseous phase is expressed in terms of phase mobilities, Eq. (A7) as

$$f = \frac{\int_0^H \frac{k(z)k_{rg}(s)dz}{\mu_g[1 + \beta_s \Delta \sigma_{cr}(s) + \beta_a a]}}{\left[\int_0^H \frac{k(z)k_{rw}(s)dz}{\mu_w} + \int_0^H \frac{k(z)k_{rg}(s)dz}{\mu_g[1 + \beta_s \Delta \sigma_{cr}(s) + \beta_a a]} \right]} = \frac{\lambda_g(s)}{[\lambda_w(s) + \lambda_g(s)]} = \frac{\lambda_g(s)}{\lambda(s)}, \quad (14)$$

The overall fractional flow of the CO₂ component is expressed as

$$F = (1 - c_w)f + (1 - f)c_g \quad (15)$$

From Eqs. (B2) and (B6), the overall gas flux (detailed derivation of which is provided in Appendix B) is obtained in terms of the overall fractional flow of CO₂ as expressed in Eq. (15) as

$$U_g = UF + [F - (1 - c_w)] \int_0^H \frac{k(z)k_{rg}(s)dz}{\mu_g[1 + \beta_s \Delta \sigma_{cr}(s) + \beta_a a]} \frac{\partial p_c(s)}{\partial r} \quad (16)$$

For thick reservoirs where the thickness H exceeds the characteristic thickness H_c of the transition zone, the averaged pseudo-functions are derived accordingly. The overall CO₂-component concentration C_g and fractional flow F calculations in such a reservoir configuration, depicted in Fig. 3a, are summarized in Table

1. Specifically, the second row of Table 1 lists the equations for overall gas saturation S_0 , CO₂ concentration C_0 , and fractional flow of the gas phase $f_0(S)$ within Zone 0, which encompasses the zone with the transition region above the brine phase. The third row presents the corresponding expressions for Zone 01, which encompasses the zone where the transition region exist between the gas and brine phases. The fourth row contains the formulas for Zone 1, where the transition region occurs below the gaseous phase. The overall fractional flows of the CO₂ component for these zones, denoted $F_0(C)$, $F_{01}(C)$, and $F_1(C_g)$, are computed using Eq. (15).

Table 1—Derived expressions for averaged gas-component concentration and fractional flux across the distinct flow regions of a thick reservoir.

Region	$S(r,t)$	Overall CO ₂ concentration $C_g = S(1 - c_w) + (1 - S)c_g$	Fractional flow for gas phase $f(S)$
0	$\frac{1}{H} \int_{z_0}^H \left(J_d + (z - z_0) \frac{\Delta \rho_g}{\sigma} \sqrt{\frac{k(z)}{\phi}} \right) dz$	$c_g + \frac{(1 - c_w - c_g)}{H} \bullet$ $\int_{z_0}^H \left(J_d + (z - z_0) \frac{\Delta \rho_g}{\sigma} \sqrt{\frac{k(z)}{\phi}} \right) dz$	$\frac{\int_{z_0}^H k(z) k_{rg}(s) dz}{\int_{z_0}^H [1 + \beta_s \Delta \sigma_{cr}(s)]}$ $\frac{\mu_g}{\mu_w} \int_0^{z_0} k(z) dz + \int_{z_0}^H \frac{k(z) k_{rg}(s) dz}{[1 + \beta_s \Delta \sigma_{cr}(s)]}$
01	$\frac{1}{H} \int_{z_0}^{z_0+H_c} s(z) dz + \frac{(H - H_c - z_0)}{H}$	$c_g + (1 - c_w - c_g) \bullet$ $\left[\frac{1}{H} \int_{z_0}^{z_0+H_c} s(z) dz + \frac{(H - H_c - z_0)}{H} \right]$	$\left[\int_{z_0}^{z_0+H_c} \frac{k(z) k_{rg}(s) dz}{[1 + \beta_s \Delta \sigma_{cr}(s)]} + \frac{k_{rgwc}}{[1 + \beta_s \Delta \sigma_{cr}(1) + \beta_a a]} \int_{z_0+H_c}^1 k(z) dz \right] \bullet$ $\left\{ \frac{\mu_g}{\mu_w} \left(\int_0^{z_0} k(z) dz + \int_{z_0}^{z_0+H_c} \frac{k_{rw}(s) k(z) dz}{\mu_w} \right) + \right.$ $\left. \int_{z_0}^{z_0+H_c} \frac{k(z) k_{rg}(s) dz}{[1 + \beta_s \Delta \sigma_{cr}(s)]} + \frac{k_{rgwc}}{[1 + \beta_s \Delta \sigma_{cr}(1) + \beta_a a]} \int_{z_0+H_c}^1 k(z) dz \right\}^{-1}$
1	$\frac{1}{H} \int_0^{z_1} \left(J_m + (z - z_1) \frac{\Delta \rho_g}{\sigma} \sqrt{\frac{k(z)}{\phi}} \right) dz + \frac{(H - z_1)}{H}$	$c_g + (1 - c_w - c_g) \bullet$ $\left\{ \frac{1}{H} \int_0^{z_1} \left(J_m + (z - z_1) \frac{\Delta \rho_g}{\sigma} \sqrt{\frac{k(z)}{\phi}} \right) dz + \frac{(H - z_1)}{H} \right\}$	$\left[\int_0^{z_1} \frac{k(z) k_{rg}(s) dz}{[1 + \beta_s \Delta \sigma_{cr}(s)]} + \frac{k_{rgwc}}{[1 + \beta_s \Delta \sigma_{cr}(1) + \beta_a a]} \int_{z_1}^1 k(z) dz \right] \bullet$ $\left\{ \frac{\mu_g}{\mu_w} \int_0^{z_1} k(z) k_{rw}(s) dz + \int_0^{z_1} \frac{k(z) k_{rg}(s) dz}{[1 + \beta_s \Delta \sigma_{cr}(s)]} + \right.$ $\left. \frac{k_{rgwc}}{[1 + \beta_s \Delta \sigma_{cr}(1) + \beta_a a]} \int_{z_1}^1 k(z) dz \right\}^{-1}$

For thin reservoirs, where the capillary transition zone is thicker than the reservoir itself (Fig. 3b), the expressions for capillary pressure, vertical saturation distribution, and gas concentration at the advancing and receding fronts remain consistent with those derived for thick reservoirs. Table 2 details the relevant equations, including overall gas saturation $S(r,t)$ in column two, CO₂ concentration in column three, and fractional flow for the gas phase $f(S)$ in column four. The second row of the table presents these expressions for Zone 0; the third row covers Zone 01; and the fourth row provides the formulas for Zone 1. The overall fractional flow of the CO₂ component as a function of its concentration, $F_1(C_g)$, is calculated using Eq. (15).

Table 2—Derived expressions for averaged gas-component concentration and fractional flux across the distinct flow regions of a thin reservoir.

Region	$S(r,t)$	Overall CO ₂ concentration $C_g = S(1 - c_w) + (1 - S)c_g$	Fractional flow for gas phase $f(S)$
0	$\frac{1}{H} \int_{z_0}^H J_0 \left(J_d + (z - z_0) \frac{\Delta \rho g}{\sigma} \sqrt{\frac{k(z)}{\phi}} \right) dz$	$\frac{(1 - c_w - c_g)}{H} \int_{z_0}^H J_0 \left(J_d + (z - z_0) \frac{\Delta \rho g}{\sigma} \sqrt{\frac{k(z)}{\phi}} \right) dz$	$\frac{\int_{z_0}^H \frac{k(z)k_{rg}(s)}{[1 + \beta_s \Delta \sigma_{cr}(s)]} dz}{\left[\frac{\mu_g}{\mu_w} \int_0^H \frac{k(z)k_{rw}(s)}{\mu_w} dz + \int_{z_0}^H \frac{k(z)k_{rg}(s)}{[1 + \beta_s \Delta \sigma_{cr}(s)]} dz \right]}$
01	$\frac{1}{H} \int_0^H s(r,t) dz$	$c_g + (1 - c_w - c_g) \frac{1}{H} \int_0^H s(r,t) dz$	$\frac{\int_0^H \frac{k(z)k_{rg}(s)}{[1 + \beta_s \Delta \sigma_{cr}(s)]} dz}{\left[\frac{\mu_g}{\mu_w} \int_0^H \frac{k(z)k_{rw}(s)}{\mu_w} dz + \int_0^H \frac{k(z)k_{rg}(s)}{[1 + \beta_s \Delta \sigma_{cr}(s)]} dz \right]}$
1	$\frac{1}{H} \int_0^{z_1} J_1 \left(J_m + (z - z_1) \frac{\Delta \rho g}{\sigma} \sqrt{\frac{k(z)}{\phi}} \right) dz + \frac{(H - z_1)}{H}$	$\frac{c_g + (1 - c_w - c_g)}{H} \int_0^{z_1} J_1 \left(J_m + (z - z_1) \frac{\Delta \rho g}{\sigma} \sqrt{\frac{k(z)}{\phi}} \right) dz + \frac{(H - z_1)}{H}$	$\left[\frac{\int_0^{z_1} \frac{k(z)k_{rg}(s)}{[1 + \beta_s \Delta \sigma_{cr}(s)]} dz}{\left[\frac{\mu_g}{\mu_w} \int_0^{z_1} \frac{k(z)k_{rw}(s)}{\mu_w} dz + \int_0^{z_1} \frac{k(z)k_{rg}(s)}{[1 + \beta_s \Delta \sigma_{cr}(s)]} dz \right]} + \frac{k_{rgwc}}{[1 + \beta_s \Delta \sigma_{cr}(1) + \beta_a a]} \int_{z_1}^H k(z) dz \right] \cdot \left[\frac{k_{rgwc}}{[1 + \beta_s \Delta \sigma_{cr}(1) + \beta_a a]} \int_{z_1}^H k(z) dz \right]^{-1}$

1D Averaged mass balance for gas and salt

The 1D governing equation describing displacement of partially miscible CO₂-brine in a heterogeneous, non-deformable layer-cake reservoir with salt precipitation and fines migration is expressed as

$$\phi \frac{\partial C_g}{\partial t} + \frac{1}{r} \frac{\partial (r U_g)}{\partial r} = 0 \quad (17)$$

$$\frac{\partial [C_s(1 - S) + A]}{\partial t} + \frac{1}{r} \frac{\partial [r C_s U(1 - F)]}{\partial r} = 0 \quad (18)$$

The initial and boundary conditions for Eqs. (17) and (18), describing the displacement of brine by CO₂, is formulated as:

$$\begin{cases} t = 0: C_g = 0, C'_s = C^0, A = 0 \\ r = r_w: C_g = C_g^*, C'_s = 0, A = A_p \end{cases} \quad (19)$$

By substituting the overall CO₂ flux expression in Eq. (16) into the mass balance Eq. (17), and introducing the dimensionless parameters defined in Eq. (B7), the displacement of brine by CO₂ in a heterogeneous layer-cake system accounting for fines migration and salt precipitation is governed by the following dimensionless system of equations:

$$\frac{\partial C_g}{\partial \tau} + \frac{\partial F}{\partial x} = -\delta \frac{\partial}{\partial x} \left[(F - (1 - c_w)) \int_0^1 \frac{K(Z)k_{rg}(s)dZ}{\mu(1 + \beta \Delta \sigma_{cr}(s) + \beta_a a)} x \frac{\partial J(s)}{\partial x} \right] \quad (20)$$

$$\frac{1}{\phi} \frac{\partial [C_s(1 - S) + A]}{\partial \tau} + \frac{\partial [C_s(1 - F)]}{\partial x} = 0 \quad (21)$$

and the associated initial and boundary conditions in dimensionless form are:

$$\begin{cases} \tau = 0: C_g = 0, C_s = 1, A = 0 \\ x = x_w = \left(\frac{r_w}{R}\right)^2: C_g = C_g^*, C_s = 0, A = A_p/C^0 \end{cases} \quad (22)$$

The flow problem with negligibly small δ corresponds to large scale approximation, that is,

$$\delta = \frac{4\pi k_0 H}{Q\mu_w} \frac{\sigma \cos\theta \sqrt{\phi}}{\sqrt{k_0}} \ll 1 \quad (23)$$

Using representative reservoir values, namely, injection rate of CO₂ $Q = 1.25\text{e-}2 \text{ m}^3/\text{s}$ into a reservoir initial saturated with brine with viscosity, $\mu_w = 1.36\text{mPas}$. Considering reservoir thickness is $H = 15\text{m}$, average absolute permeability, $k_o = 3.5\text{e-}13\text{m}^2$; contact angle, $\theta = 30^\circ$; interfacial tension $\sigma = 20\text{mN/m}$; it is determined that the value of δ is negligibly small ($\delta \approx 0.08 \ll 1$). Therefore, applying large-scale approximation to the conservation law for gas Eq. (20) yields

$$\frac{\partial C_g}{\partial \tau} + \frac{dF}{dC_g} \frac{\partial C_g}{\partial x} = 0 \quad (24)$$

where the second term in Eq. (24) is obtained by applying the chain rule.

Exact analytical solution

The 1D hyperbolic equation (24) allows for an exact solution constrained by the conditions Eq. (22). In this section, the solution to the flow problem is derived in terms of the self-similar variable,

$$\xi = \frac{x}{\tau}, \quad \begin{cases} \partial x = \tau \partial \xi \\ \partial \tau = -\tau / \xi \partial \xi \end{cases} \quad (25)$$

The exact solution to Eq. (20) under conditions given by Eq. (22) is expressed in terms of the self-similar variable, $\xi = x/\tau$ as

$$C_g(\xi) = \begin{cases} 1, & \frac{x_w}{\tau} < \xi < D_1 \\ \xi = \frac{x}{\tau} = F(C_g), & D_1 < \xi < D_0 \\ 0, & D_0 < \xi < \infty \end{cases} \quad (26)$$

The mass balance (Hugoniot-Rankine) conditions on the shock fronts z_0 and z_1 require that the shock velocities at the advancing and receding fronts satisfy the conservation of mass across these discontinuities. Specifically, the shock velocities at the advancing and receding front are given as the ratio of the difference in fluxes to the difference in concentrations across the shock front.

$$\frac{dx}{d\tau}(z_0) = D_0 = \frac{F(C_g^+) - F(C_g^-)}{C_g^+ - C_g^-} = \frac{F(C_g^-)}{C_g^-}, \quad \frac{dx}{d\tau}(z_1) = D_1 = \frac{F(C_g^+) - F(C_g^-)}{C_g^+ - C_g^-} = \frac{F(C_g^+) - 1}{C_g^+ - 1} \quad (27)$$

Also, the Hugoniot-Rankine condition of mass balance of salt across the receding shock front at z_0 is

$$[C_s^+(1 - S^+) + A^+ - C_s^-(1 - S^-) - A^-]D_1 = [C_s^+(1 - F^+) - C_s^-(1 - F^-)]\phi \quad (28)$$

Assuming full dry-out of water and instantaneous salt precipitation at the receding front, the concentration of precipitated salt is obtained from Eq. (26) as

$$A^- = (1 - S^+) - \frac{(1 - F^+)\phi}{D_1} \quad (29)$$

Fig. 4 illustrates a typical fractional flow curve for a binary mixture of brine and CO₂ that incorporates partial miscibility effects between the two fluids. This curve reflects how the fractional flow varies as a function of the system variables, accounting for CO₂ dissolution in brine and brine vaporization into CO₂. The figure also demonstrates the nature of the self-similar solution expressed in terms of the similarity variable ξ , which characterizes the spatial-temporal evolution of the displacement process under partial

miscibility conditions. This self-similar solution allows for graphical interpretation of displacement fronts and phase concentrations pertinent to CO₂-brine flow in porous media.

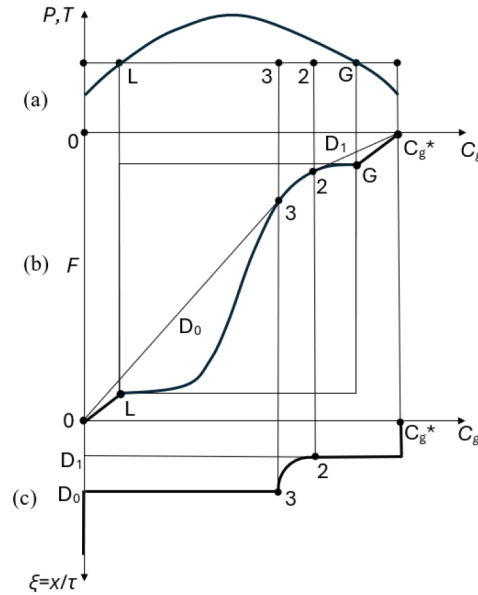


Figure 4—Fractional-flow formulation accounting for partial miscibility between brine and CO₂: (a) phase diagram showing pressure–temperature dependence on overall CO₂ concentration in the gaseous and aqueous phases; (b) total CO₂ flux, expressed as the sum of phase-specific fluxes, as a function of overall CO₂ concentration; (c) self-similar solution for total CO₂ concentration plotted against propagation speed v .

Pressure distribution in the reservoir

Condition of low compressibility ahead of the displacement front. This section demonstrates that the two-dimensional single-phase flow of a low-compressibility fluid ahead of the advancing displacement front can be averaged over the vertical coordinate z , resulting in the classical one-dimensional pressure-diffusivity equation. The governing two-dimensional mass balance equation for low-compressible brine ahead of the advancing front is given as

$$\frac{\partial}{\partial t}(\phi \rho_w) + \frac{1}{r} \frac{\partial}{\partial r}(r \rho_w u_{wr}) + \frac{\partial}{\partial z}(\rho_w u_{wz}) = 0 \quad (30)$$

Assuming hydrostatic pressure distribution and low compressibility of the rock-brine system, the pressure diffusivity equation can be written as:

$$\frac{\partial P}{\partial \tau} = \kappa \frac{\partial}{\partial x} \left(x \frac{\partial P}{\partial x} \right) \quad (31)$$

where κ is the pressure-diffusivity coefficient associated with the averaged permeability (Eq. (C4)) and P represents the depth-averaged reservoir pressure. The detailed derivation is provided in Appendix C.

By setting the advancing front flux equal to the injection rate and fixing far-field pressure equal to initial reservoir pressure, Eq. (30) is governed by the following boundary conditions:

$$\begin{cases} r = r_f(z_0), Q = Q_{inj} \\ P(\infty) = P_e \end{cases} \quad (32)$$

Introducing the dimensionless parameters in Eq. (B7) together with the self-similar variable defined in Eq. (25) into Eq. (32) results in:

$$\begin{cases} \xi = D_0, Q = Q_{inj} \rightarrow \frac{\partial P}{\partial x} = -\frac{1}{\Lambda(S=0)x} \\ P(\infty) = P_e \end{cases} \quad (33)$$

By applying the boundary conditions in Eq. (33) to Eq. (31), the pressure distribution ahead of the brine-gas front, accounting for low brine compressibility, is obtained as (see Appendix C):

$$P = -\frac{1}{\Lambda(0)} e^{\left(\frac{D_0}{\kappa}\right)} Ei\left(-\frac{\xi}{\kappa}\right) + P_e \quad (34)$$

Calculations of total mobility in two-phase region

The overall flux, defined as the sum the averaged gas and brine fluxes is expressed in Eq. (B2). Applying the assumption of large-scale approximation and introducing the dimensionless parameters Eq. (B7) yields the following dimensionless form:

$$1 = -\Lambda(S)x \frac{\partial P}{\partial x} \quad (35)$$

where the total mobility is generally defined as

$$\Lambda(S) = \left[\int_0^1 \frac{K(Z)k_{rg}(s)}{[1 + \beta\Delta\sigma_{cr}(s) + \beta_a a]} dZ - \frac{\mu_g}{\mu_w} \int_0^1 K(Z)k_{rw}(s) dZ \right] \quad (36)$$

The detailed derivation of expression for the total mobility of phases in Zone 0, Zone 01 and Zone 1 are given by Eqs. (D5-D7) in Appendix D.

Sensitivity study

This section presents the sensitivity analysis of brine displacement by injected CO₂, evaluating the effects of reservoir heterogeneity, viscosity ratio, formation damage coefficient, and concentration of detachable fines, while simultaneously varying the humidity of the injected CO₂. The colour scheme is as follows: blue denotes CO₂ injected at equilibrium vapour concentration ($C_g = C_g$ equilibrium), red corresponds to humid CO₂ ($C_g = C_g^*$), and yellow represents dry CO₂ ($C_g = I$) respectively.

The analysis begins with a layer-cake reservoir exhibiting depth-varying permeability, where $k(z)$ is prescribed as a third-order polynomial function

$$k(z) = (k_{\max} - k_{\min})\left(\frac{z}{H}\right)^3 + k_{\min} \rightarrow k(Z) = (k_{\max} - k_{\min})Z^3 + k_{\min} \quad (37)$$

The permeability distribution spans $k_{\min} = 2mD$ to $k_{\max} = 700mD$. We consider a reservoir of thickness, $H=25m$, reservoir pressure of $P_e=400bars$ and temperature of $180^\circ C$. Based on the work of Coelho et al. 2025, we set the equilibrium concentrations of CO₂ in the gas and aqueous phases are $c_g = 0.03$, $c_w = 0.09$, respectively. The salinity of the brine is fixed at 1.09 mol.kg^{-1} . Capillary pressure is represented by a Leverett-type function, and phase flow properties are described using Corey relative permeability curves as follows:

$$J(s) = C(s)^{-\eta}, k_{rg}(s) = k_{rgwi}(s)^{n_g}, k_{rw}(s) = k_{rwwr}(s)^{n_w} \quad (38)$$

The end point relative permeability of gas and brine are $k_{rgwi} = 0.6$ and $k_{rwwr} = 1$ respectively at end point saturations of gas and brine given as 0 and 0.2, respectively. The fluid exponents for gas and brine are $n_g = 3$ and $n_w = 5$ and the Corey index is $\eta = 1.3$. Formation-damage behaviour due to fines migration is described using the following parameter values: total detachable fines concentration on the rock surface, $\sigma(I) = 7.12 \times 10^{-4}$; power law exponent for straining, $B = 1.73$; and the formation damage coefficient, $\beta = 1.5 \times 10^4$.

Effects of heterogeneity

We use the relative range, v , which is defined as the difference between the maximum and minimum permeability divided by the mean permeability. This relative range quantifies the spread of permeability values relative to the average; a higher relative range indicates greater heterogeneity, while a lower relative

range suggests more uniform permeability, as shown in Fig. 5a. As the reservoir heterogeneity increases, both the fractional flow and the concavity of the fractional flow curve increase, which consequently results in a higher gas cut (Fig. 5b). Fig. 5b-d further show that increasing heterogeneity reduces the breakthrough period from 0.37 PVI to 0.2 PVI regardless of humidity levels. Additionally, greater heterogeneity extends the evaporation period, which is most pronounced for dry CO₂ injection and least for CO₂ injected at equilibrium. Increased heterogeneity also lowers sweep efficiency and reduces stabilized impedance, with the strongest effects observed for dry CO₂ injection and the weakest under equilibrium conditions. Humid CO₂ injection exhibits behaviour between these two extremes.

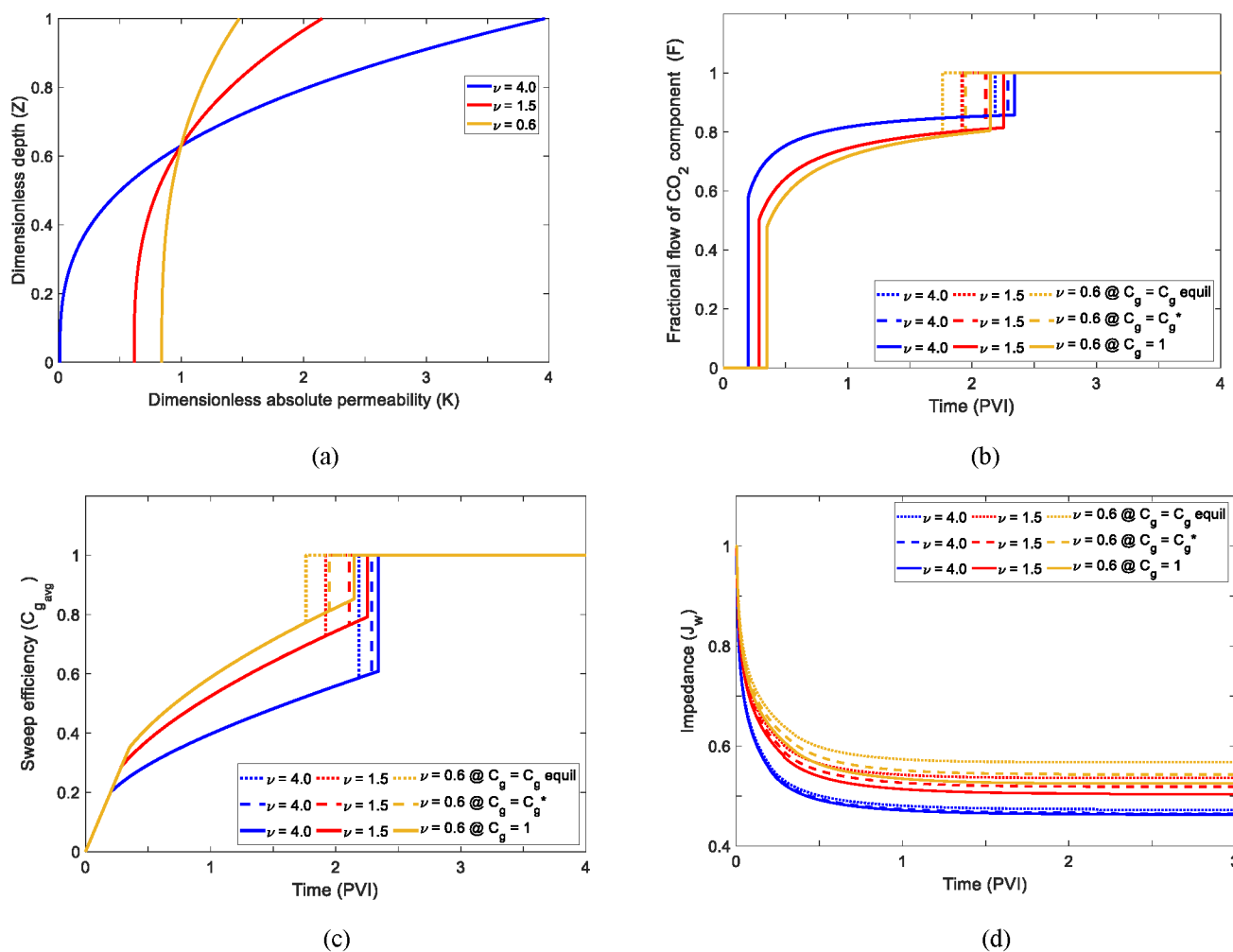


Figure 5—Effect of reservoir heterogeneity on CO₂ injection into brine at varying humidity levels: (a) dimensionless permeability profile with depth, Z; (b) CO₂ fractional-flow history at the outlet; (c) sweep efficiency as a function of time; (d) impedance evolution during injection.

Effects of viscosity ratio

Fig. 6 shows the effect of different gas-to-brine viscosity ratios, $\mu = \mu_g/\mu_w$ on brine displacement by CO₂. In this analysis, the viscosity ratio ranges from 0.021– representative of gaseous CO₂ to 0.1, typical of supercritical CO₂. Fig. 6a presents the breakthrough gas cuts ($F(C_g)$) versus time (PVI) at the outlet $x = l$, showing that higher viscosity ratios result in a lower gas fraction at the outlet irrespective of the degree of humidity. As a result, higher viscosity ratios lead to improved sweep efficiency (Fig. 6b) while independent of the humidity level. Here, the time of arrival of the receding front is slower for dry gas injection compared to the injection of CO₂ at equilibrium conditions. Also, the stabilized well impedance approximately doubles

with increasing viscosity ratio (Fig. 6c). For each given viscosity ratio, the impedance is marginally higher for gas injection at equilibrium conditions than dry gas injection.

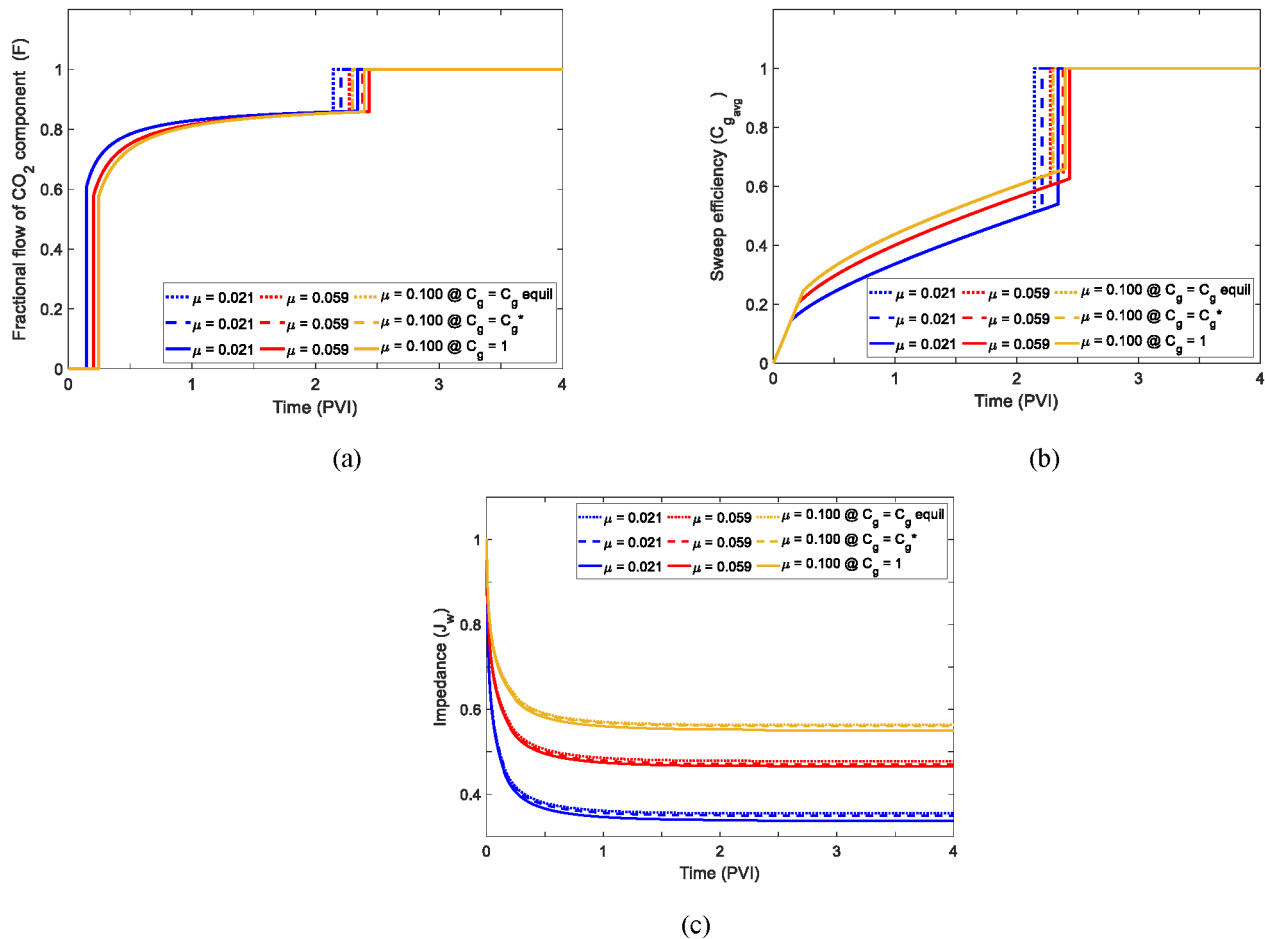


Figure 6—Effect of viscosity ratio on CO₂ injection into brine at varying humidity levels: (a) CO₂ fractional-flow history at the outlet; (b) sweep efficiency as a function of time; (c) impedance evolution during injection.

Effects of formation damage coefficient

Fig. 7a illustrates that increasing the formation damage coefficient from zero to 30,000 extends the breakthrough period, while shortening the evaporation period for a given humidity level. The time arrival of the receding front at the outlet is however greater for humid CO₂, followed by dry CO₂ and CO₂ at equilibrium conditions. Furthermore, as depicted in Fig. 7b, this increase in β results in a significant improvement in sweep efficiency. Also, higher β results in increased the stabilized impedance at every given condition of injected CO₂. The impedance is marginally higher for gas injection at equilibrium conditions than dry gas injection.

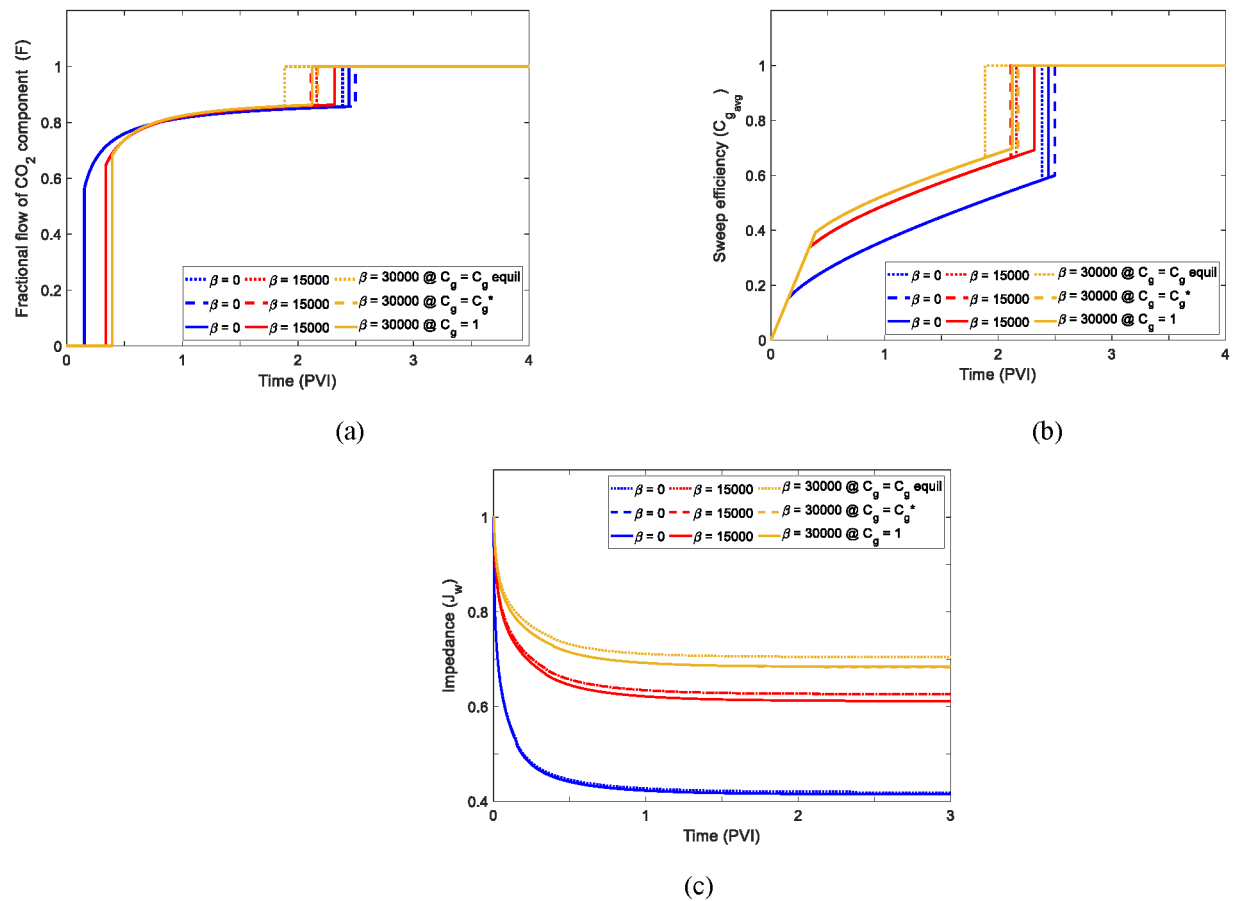


Figure 7—Effect of damage coefficient on CO₂ injection into brine at varying humidity levels: (a) CO₂ fractional-flow history at the outlet; (b) sweep efficiency as a function of time; (c) impedance evolution during injection.

Effects of total detachable fines concentration on rock surface

Fig 8 illustrates the impact of the total concentration of detachable fines. As this concentration increases, so does the amount of strained fines, leading to greater formation damage in the gas phase and a corresponding deceleration of gas flow. Fig 8 shows that increasing $\sigma(1)$ extends the breakthrough time and shortens the evaporation period at all humidity level. The shortening of the evaporation period is non-monotonic when the level of humidity in injected CO₂ is considered. While sweep efficiency improves as $\sigma(1)$ increases from 5×10^{-5} to 4.1×10^{-3} (Fig 8b), the variation of humidity levels causes no change in sweep efficiency at early times. From Fig. 8c increasing the fines concentration also leads to higher impedance, where impedance values are marginally higher for gas injection at equilibrium conditions than dry gas injection.

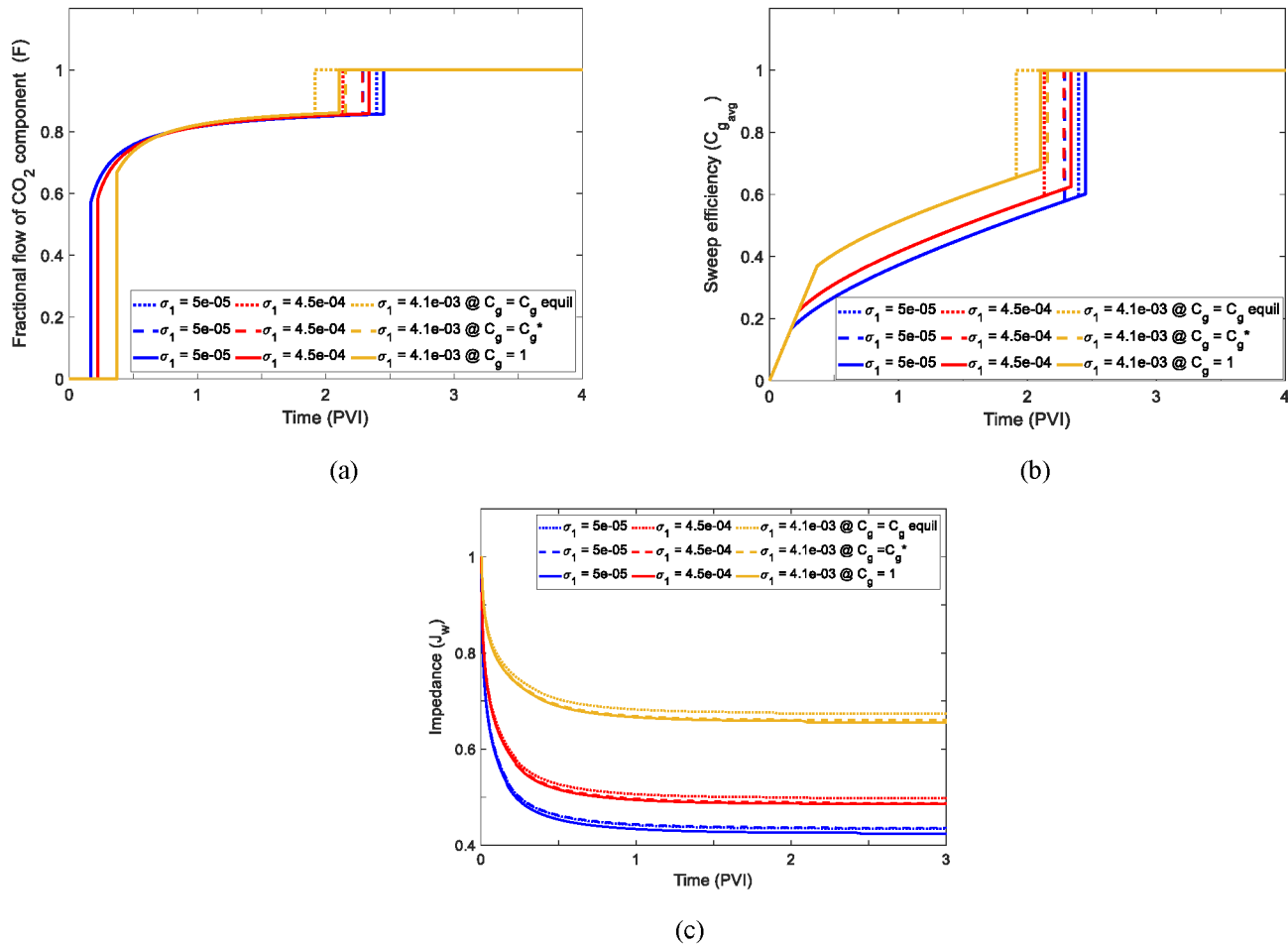


Figure 8—Effect of total detachable fines on rock surface on CO₂ injection into brine at varying humidity levels: (a) CO₂ fractional-flow history at the outlet; (b) sweep efficiency as a function of time; (c) impedance evolution during injection.

Discussion

This study developed an extended Vertical Equilibrium (VE) analytical model to describe brine displacement by CO₂ in layer-cake aquifers, accounting simultaneously for partial CO₂-brine miscibility, humidity level of injected CO₂, formation damage induced by fines-migration and salt precipitation. The model yields exact analytical expressions for averaged saturations, concentration of CO₂, sweep efficiency, and well impedance. A thorough sensitivity study is performed to evaluate the effects of reservoir heterogeneity, humidity level in injected CO₂, viscosity ratio, fines concentration, and formation damage coefficient on displacement efficiency and well injectivity. The key findings and the broader implications of the model are summarised and discussed below.

The validity of the VE assumption underlying the model has been rigorously established. Prior theoretical analyses and 2D/3D reservoir-scale simulations by Yortsos (1995) and by Yuan and Shapiro (2011) demonstrate that vertical equilibrium is achieved under a broad spectrum of conditions for immiscible displacement in layered systems. Furthermore, the maximum-retention function used to describe fines detachment arises directly from exact pore- to core-scale upscaling (Russell et al., 2025). The assumptions of instantaneous fines straining and local thermodynamic equilibrium between CO₂ and brine are justified by the much shorter characteristic relaxation times compared with the duration of one pore-volume injection (PVI). Consequently, extending the VE model to include miscibility, humidity effects, and fines migration introduces no additional conceptual restrictions beyond those inherent to classical VE formulations.

The sensitivity study reveals several influencing factors with direct implications for field CO₂ injection. It is determined that high variability of heterogeneity increases fractional flow of gas resulting to high gas cut and reduced breakthrough time coupled with prolonged evaporation period. Sweep efficiency and stabilised impedance both decline as the relative range of heterogeneity increases, with the strongest impact observed for dry CO₂, followed by humid CO₂, and the mildest effects under equilibrium CO₂ injection. These trends suggest that heterogeneity amplifies sensitivity to CO₂ humidity.

Higher viscosity ratios (from gaseous to supercritical CO₂) reduce the fractional flow of gas and significantly improve sweep efficiency. In all humidity cases, increased viscosity ratio increased the stabilised impedance. These findings emphasize the benefit of injecting denser, higher-viscosity CO₂ streams for improved sweep.

Larger β delays breakthrough but shortens the evaporation period. Sweep efficiency increases substantially with β , while stabilised impedance rises across all humidity levels. The receding front reaches the outlet late for humid CO₂, followed by dry CO₂, and earliest for equilibrium CO₂. This indicates a strong coupling between fines-migration kinetics, humidity-controlled evaporation, and flow resistance. Also, increasing fines concentration increases straining, reduces gas mobility, extends breakthrough time, and shortens evaporation duration. Sweep efficiency improves with $\sigma(1)$, particularly at late times, whereas early-time sweep is nearly insensitive to humidity. Impedance increases with $\sigma(1)$ with slightly higher values for equilibrium CO₂. These results highlight the dual role of fines migration, that is, injectivity is impaired but sweep is improved due to the reduction of gas-phase mobility. Across all the parameters tested, CO₂ humidity consistently influenced the severity of evaporation, salt precipitation, and fines migration.

The larger scale VE model (Eq. 24) presented in this study does not explicitly include capillary pressure, which plays an important role in saturation distribution and transition-zone thickness. Incorporating capillarity will enlarge the physically admissible space of displacement regimes and allow an exact self-similar solution for Eq. (20) where initial saturation is reached asymptotically as radius approaches infinity. This extension is an active direction of further research.

Conclusions

This study advances the classical VE framework by incorporating partial CO₂-brine miscibility, humidity of the injected CO₂ stream, and formation damage associated with fines migration and salt precipitation. Vertical averaging of the microscale CO₂ concentration leads to a radial, quasi-2D analytical model that governs brine displacement by CO₂ in stratified (layer-cake) aquifers. At the reservoir scale, the resulting formulation admits an exact self-similar solution and yields closed-form expressions for saturation profiles, CO₂ concentration, sweep efficiency, and well injectivity. Additionally, the pressure $p(r,t)$ in the incompressible flow region is matched continuously to the initial reservoir pressure by imposing the condition of slight compressibility of brine ahead of the displacement or advanced front. This enables the continuity of pressure across the flow domain.

The results show that reservoir heterogeneity, viscosity ratio, fines migration, and CO₂ humidity collectively exert strong influence over displacement dynamics. Increasing heterogeneity accelerates breakthrough, lengthens the evaporation period, and reduces both sweep efficiency and stabilised impedance, with the strongest deterioration observed for dry CO₂. Higher viscosity ratios improve sweep and increase impedance regardless of humidity. Increased fines concentration and formation damage delay gas breakthrough, shorten the evaporation period, enhance sweep efficiency, and raise impedance.

Overall, the extended VE model offers a fast and robust tool for assessing injectivity and storage capacity under coupled miscibility, evaporation, and fines-migration effects, providing clear guidance for optimising CO₂ injection strategies in layer cake aquifers.

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Nomenclature

a	Microscale adsorbed or precipitated salt concentration, [-]
A	Adsorbed or precipitated salt concentration, [-]
B	Power law exponent for straining, [-]
C_g	Overall CO ₂ component concentration, [-]
$\tilde{C}_g$	CO ₂ component at the microscale, [-]
c_t	Total compressibility, [ML ⁻¹ T ⁻²]
f	Fractional flow of gas, [-]
f_o	Fractional flow of gas in zone 0, [-]
f_{01}	Fractional flow of gas in zone 01, [-]
f_1	Fractional flow of gas in zone 1, [-]
F	Overall fractional flow of CO ₂ component
g	Gravitational acceleration, [LT ⁻²]
H	Total height of reservoir, [L]
h_c	Dimensionless height of transition zone, [-]
J	Leverett J function, [-]
J_w	Well Impedance, [-]
j	Inverse of Leverett function, [-]
$k(z)$	Horizontal permeability as a function of depth, [L ²]
$k(Z)$	Horizontal permeability as a function of dimensionless depth, [L ²]
$K(Z)$	Dimensionless horizontal permeability as a function of dimensionless depth, [-]
k_{min}	Minimum permeability, [L ²]
k_{max}	Maximum permeability, [L ²]
k_0	Average permeability, [L ²]
k_{rg}	Gas relative permeability, [-]
k_{rw}	Brine relative permeability, [-]
k_{rgwi}	End point gas relative permeability, [-]
k_{rwgr}	End point brine relative permeability, [-]
n_g	Corey fluid index for gas, [-]
n_w	Corey fluid index for brine, [-]
p	Pressure, [ML ⁻¹ T ⁻²]
$\tilde{p}$	Microscale pressure, [ML ⁻¹ T ⁻²]
P	Dimensionless pressure, [-]
p_c	Capillary pressure [ML ⁻¹ T ⁻²]
p_d	Capillary pressure in brine filled region [ML ⁻¹ T ⁻²]
p_e	Reservoir pressure, [ML ⁻¹ T ⁻²]
p_m	Capillary pressure in gas filled region [ML ⁻¹ T ⁻²]
P_e	Dimensionless reservoir pressure, [-]
Q	Rate, [L ³ T ⁻¹]
r	Radial coordinate, [L]
r_w	Well radius, [L]

R	Drainage radius, [L]
S	Averaged gas saturation, [-]
s^*	Microscale gas saturation, [-]
s	Normalized microscale gas saturation, [-]
S_0	Averaged gas saturation in zone 0, [-]
S_{0l}	Averaged gas saturation in zone 0l, [-]
S_l	Averaged gas saturation in zone 1, [-]
t	Time, [T]
τ	Dimensionless time [-]
U	Total flux, [LT ⁻¹]
U_g	Overall CO ₂ component flux, [LT ⁻¹]
U_{gr}^*	Radial gas flux, [LT ⁻¹]
U_{wr}^*	Radial brine flux, [LT ⁻¹]
U_{wr}	Overall radial brine flux, [LT ⁻¹]
U_{wz}	Overall vertical brine flux, [LT ⁻¹]
$\hat{u}_{gr}$	Radial microscale gas flux, [LT ⁻¹]
$\hat{u}_{gz}$	Vertical microscale gas flux, [LT ⁻¹]
x	Dimensionless length, [-]
x_w	Dimensionless well length, [-]
z	Depth, [L]
Z	Dimensionless depth, [-]
z_0	Position of the advanced front, [L]
z_l	Position of the receded front, [L]
ΔP	Dimensionless pressure drops, [-]

Greek Symbols

β_s	Formation damage coefficient due to fines migration, [-]
β_a	Formation damage coefficient due to salt precipitation, [-]
ϕ	Porosity, [-]
μ	Gas-brine viscosity ratio, [-]
μ_g	Gas viscosity, [ML ⁻¹ T ⁻¹]
μ_w	Brine viscosity, [ML ⁻¹ T ⁻¹]
ρ_G	CO ₂ density, [ML ⁻³]
ρ_g	Gaseous phase density, [ML ⁻³]
ρ_w	Brine density, [ML ⁻³]
ρ_w	Aqueous phase density, [ML ⁻³]
κ	Pressure-diffusivity coefficient
ζ	Self-similar variable, [-]
σ_0	Initial fines concentration, [-]
σ_s	Strained fines concentration, [-]
γ	Dimensionless parameter, [-]
λ	Total mobility, [M ⁻¹ L ³ T]
λ_g	Gas mobility, [M ⁻¹ L ³ T]
λ_w	Brine mobility, [M ⁻¹ L ³ T]
Λ	Dimensionless total mobility,
v	Relative range for permeability heterogeneity, [-]

η Corey index for Leverett function, [-]

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Appendix A

Vertical phase distribution under hydrostatic pressure

Taking the difference of the hydrostatic pressure expressions in Eq. (3) leads directly to the first-order derivative for capillary pressure, expressed as

$$\frac{dp_c}{dz} = \Delta\rho g, \quad \Delta\rho = \rho_w - \rho_g \quad (\text{A1})$$

The gas saturation and capillary pressure at the advanced front, z_0 and the receded front, z_l are given respectively by

$$z = z_0(x, t): \quad s = 0, \quad p_c = p_d \quad (\text{A2})$$

$$z = z_l(x, t): \quad s = 1, \quad p_c = p_m \quad (\text{A3})$$

Integrating Eq. (A1) gives

$$p_c(z) = \Delta\rho g z + \text{const} \quad (\text{A4})$$

Substituting Eqs. (A2) and (A3) into Eq. (A4) and taking the difference of the resulting expressions yields the thickness of the capillary transition zone, H_c .

$$p_m - p_d = \Delta\rho g H_c, \quad H_c = z_l - z_0 \quad (\text{A5})$$

Next, integrating Eq. (A1) from z to z_0 , while applying the boundary condition in Eq. (A2) gives the capillary pressure at the advanced front:

$$p_c(s) - p_d = \Delta\rho g(z - z_0) = \frac{\sigma[J(s) - J_d]}{\sqrt{k(z)/\phi}}, \quad J(s) = J_d + (z - z_0) \frac{\Delta\rho g}{\sigma} \sqrt{k(z)/\phi} \quad (\text{A6})$$

Using the inverse of Eq. (A6), $j = J^{-1}$, the vertical saturation distribution within the two-phase zone is obtained as

$$s = j\left(J_d + (z - z_0) \frac{\Delta\rho g}{\sigma} \sqrt{k(z)/\phi}\right) \quad (\text{A7})$$

Substituting Eq. (A7) into the first relation in Eq. (2) gives the gas concentration at the bottom of the two-phase zone, evaluated at $z=z_0$:

$$\tilde{c}_g = j\left(J_d + (z - z_0) \frac{\Delta\rho g}{\sigma} \sqrt{k(z)/\phi}\right) (1 - c_w - c_g) + c_g \quad (\text{A8})$$

Similarly, integrating Eq. (A1) from z to z_l , and incorporating Eq. (A3) gives the corresponding expression for the capillary pressure at the receding front:

$$p_c(s) - p_m = \Delta\rho g(z - z_l) = \frac{\sigma[J(s) - J_m]}{\sqrt{k(z)/\phi}}, \quad J(s) = J_m + (z - z_l) \frac{\Delta\rho g}{\sigma} \sqrt{k(z)/\phi} \quad (\text{A9})$$

Finally, substituting the inverse function for Eq. (A9) into Eq. (2) yields the gas concentration at the upper boundary of the two-phase zone, evaluated at $z=z_l$:

$$\tilde{c}_g = j\left(J_m + (z - z_l) \frac{\Delta\rho g}{\sigma} \sqrt{k(z)/\phi}\right) (1 - c_w - c_g) + c_g \quad (\text{A10})$$

Appendix B

Total Phase Fluxes

The upscaled phase fluxes of brine and gas in the radial direction are obtained by integrating Eq. (11) across the reservoir thickness:

$$U_{wr}^* = \int_0^H u_{wr} dz = - \int_0^H \frac{k(z)k_{rw}(s)dz}{\mu_w} \frac{\partial p_w}{\partial r}, \quad U_{gr}^* = \int_0^H u_{gr} dz = - \int_0^H \frac{k(z)k_{rg}(s)dz}{\mu_g[1 + \beta\Delta\sigma_{cr}(s) + \beta_a a]} \frac{\partial p_g}{\partial r} \quad (B1)$$

By summing the phase velocities in Eq. (B1) and rewriting the resulting expression in terms of the brine pressure and capillary pressure, we obtain

$$U = - \left[\int_0^H \frac{k(z)k_{rw}(s)dz}{\mu_w} + \int_0^H \frac{k(z)k_{rg}(s)dz}{\mu_g[1 + \beta\Delta\sigma_{cr}(s) + \beta_a a]} \right] \frac{\partial p_w}{\partial r} - \int_0^H \frac{k(z)k_{rg}(s)dz}{\mu_g[1 + \beta\Delta\sigma_{cr}(s) + \beta_a a]} \frac{\partial p_c(s)}{\partial r} \quad (B2)$$

Considering the upscaled gas flux, Eq. (B1) and the first relation of Eq. (2), the overall flux of the CO₂ component is obtained as

$$U_g = -(1 - c_w) \int_0^H \frac{k(z)k_{rg}(s)dz}{\mu_g[1 + \beta\Delta\sigma_{cr}(s) + \beta_a a]} \frac{\partial p_g}{\partial r} - c_g \int_0^H \frac{k(z)k_{rw}(s)dz}{\mu_w} \frac{\partial p_w}{\partial r} \quad (B3)$$

Rearranging Eq. (B3) to express it in terms of brine-pressure and capillary-pressure yields

$$U_g = - \left[(1 - c_w) \int_0^H \frac{k(z)k_{rg}(s)dz}{\mu_g[1 + \beta\Delta\sigma_{cr}(s) + \beta_a a]} + c_g \int_0^H \frac{k(z)k_{rw}(s)dz}{\mu_w} \right] \frac{\partial p_w}{\partial r} - (1 - c_w) \int_0^H \frac{k(z)k_{rg}(s)dz}{\mu_g[1 + \beta\Delta\sigma_{cr}(s) + \beta_a a]} \frac{\partial p_c(s)}{\partial r} \quad (B4)$$

Solving Eq. (B4) for the brine pressure gradient and substituting the resulting expression into Eq. (B3) yields the overall flux of the CO₂ component as

$$U_g = \frac{(1 - c_w)\lambda_g(s) + c_g\lambda_w(s)}{\lambda(s)} U + \left\{ \frac{(1 - c_w)\lambda_g(s) + c_g\lambda_w(s)}{\lambda(s)} \lambda_g(s) - (1 - c_w)\lambda_g(s) \right\} \frac{\partial p_c(s)}{\partial r} \quad (B5)$$

Here, the gas, brine, and total mobilities are defined, respectively, as

$$\lambda_g(s) = \int_0^H \frac{k(z)k_{rg}(s)dz}{\mu_g[1 + \beta\Delta\sigma_{cr}(s) + \beta_a a]}, \quad \lambda_w(s) = \int_0^H \frac{k(z)k_{rw}(s)dz}{\mu_w}, \quad \lambda(s) = \lambda_g(s) + \lambda_w(s) \quad (B6)$$

Equations (B2)–(B6) form the basis for the derivation of the averaged mass-balance equation (15) across the three flow regions associated with thin and thick reservoir systems. To proceed, we introduce the following dimensionless variables and parameters:

$$\begin{aligned} x &= \frac{r^2}{R^2}, \quad Z = \frac{z}{H}, \quad \tau = \frac{Q\mu_w}{\phi\pi R^2}, \quad h_c = \frac{H_c}{H}, \quad \delta = \frac{4\pi k_0 H}{Q\mu_w} \frac{\sigma \cos\theta \sqrt{\phi}}{\sqrt{k_0}}, \quad \kappa = \frac{4\pi k_0}{Qc_t\mu_w}, \quad p = \frac{1}{H} \int_0^H \bar{p}(x, z, t) dz \\ P &= \frac{4\pi k_0 H}{Q\mu_w} p, \quad P_w = \frac{4\pi k_0 H}{Q\mu_w} p_w, \quad k_0 = \frac{1}{H} \int_0^H k(z) dz = \int_0^1 k(Z) dZ, \quad k(Z) = k_0 K(Z), \quad \int_0^1 K(Z) dZ = 1 \\ C_s &= \frac{C_s}{C_0}, \quad A = \frac{A}{C_0} \end{aligned} \quad (B7)$$

Appendix C

Pressure Distribution Ahead of the Advanced Front Accounting for Brine Compressibility Effects

Formulation of problem

We demonstrate here that two-dimensional single-phase, low-compressible flow under vertical gravity equilibrium can be vertically averaged to yield the classical one-dimensional pressure-diffusivity equation. The 2D mass-balance equation for low-compressible brine ahead of the advancing front is

$$\frac{\partial}{\partial t}(\phi \rho_w) + \frac{1}{r} \frac{\partial}{\partial r}(r \rho_w u_{wr}) + \frac{\partial}{\partial z}(\rho_w u_{wz}) = 0 \quad (C1)$$

Under vertical equilibrium conditions, the vertical brine velocity u_{wz} is zero. Therefore, Eq. (C1) simplifies to

$$\frac{\partial}{\partial t}(\phi \rho_w) + \frac{1}{r} \frac{\partial}{\partial r}(r \rho_w u_{wr}) = 0 \quad (C2)$$

Substituting the total compressibility from Eq. (8) and the Darcy law for brine from Eq. (11) into Eq. (C2), and neglecting the pressure dependence of brine density in the mass-transfer term, yields

$$c_t \phi_0 \frac{\partial p}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{k(z)}{\mu_w} \frac{\partial p}{\partial r} \right) \quad (C3)$$

In this form, z acts as a parameter. Considering the solution at the base of the flow domain, $p(r, 0, t)$ at $z = 0$, Eq. (C3) becomes

$$\frac{\partial p}{\partial t} = \frac{1}{H c_t \phi_0 \mu_w} \frac{1}{r} \frac{\partial}{\partial r} \left(r \int_0^H k(z) dz \frac{\partial p}{\partial r} \right) \quad (C4)$$

The quasi-2D solution is then extended from $z = 0$ to $0 < z < 1$ by using the hydrostatic relation.

Solution of pressure diffusivity equation

Introducing the dimensionless variables and parameters, including the definition of average pressure p from Eq. (B7), into Eq. (C4) yields the dimensionless pressure-diffusivity equation:

$$\frac{\partial}{\partial x} \left(x \frac{\partial P}{\partial x} \right) = \frac{1}{\kappa} \frac{\partial P}{\partial \tau} \quad (C5)$$

Applying the self-similar transformation in Eq. (25) to Eq. (C5) transforms the equation into a second-order ordinary differential form:

$$\frac{dP}{d\xi} + \xi \frac{d^2 P}{d\xi^2} = -\frac{\xi}{\kappa} \frac{dP}{d\xi} \quad (C6)$$

The order of Eq. (C6) is reduced by defining an auxiliary variable, $\omega = \frac{dP}{d\xi}$, yielding

$$\omega \left(1 + \frac{\xi}{\kappa} \right) = -\xi \frac{d\omega}{d\xi} \quad (C7)$$

Integrating both sides of Eq. (C7) using separation of variables gives

$$-\ln(\omega) = \ln(\xi) + \frac{\xi}{\kappa} + c_1 \Rightarrow \frac{dP}{d\xi} = \frac{c_1}{\xi} e^{\left(-\frac{\xi}{\kappa}\right)} \quad (C8)$$

Hence, the general solution of the ODE in Eq. (C6) is

$$P = c_1 E i \left(-\frac{\xi}{\kappa} \right) + c_2 \quad (C9)$$

where c_1 and c_2 denote the constants of integration.

Appendix D

Total Phase Mobility

Summing the overall gas and brine velocities from Eq. (B1) gives

$$2\pi r U = Q = - \left[\int_0^H \frac{k(z)k_{rw}(s)dz}{\mu_w} + \int_0^H \frac{k(z)k_{rg}(s)dz}{\mu_g[1 + \beta\Delta\sigma_{cr}(s) + \beta_a a]} \right] 2\pi r \frac{\partial p_w}{\partial r} - \int_0^H \frac{k(z)k_{rg}(s)dz}{\mu_g[1 + \beta\Delta\sigma_{cr}(s) + \beta_a a]} 2\pi r \frac{\partial p_c(s)}{\partial r} \quad (D1)$$

Substituting the dimensionless quantities defined in Eq. (B7) into Eq. (D1) yields

$$1 = - \left[\int_0^1 K(Z)k_{rw}(s)dZ + \int_0^1 \frac{K(Z)k_{rg}(s)dZ}{\mu[1 + \beta\Delta\sigma_{cr}(s) + \beta_a a]} \right] x \frac{\partial P_w}{\partial x} - \delta \int_0^1 \frac{K(Z)k_{rg}(s)dZ}{\mu[1 + \beta\Delta\sigma_{cr}(s) + \beta_a a]} x \frac{\partial J(s)}{\partial x} \quad (D2)$$

For large-scale systems where $\delta \ll 1$, the pressure drops in the gas and brine phases become equal, such that

$$\frac{\partial P_g}{\partial x} = \frac{\partial P_w}{\partial x} = \frac{\partial P}{\partial x} \quad (D3)$$

Using Eq. (D2) under this approximation, the expression for the total flux becomes

$$1 = - \left[\int_0^1 K(Z)k_{rw}(s)dZ + \int_0^1 \frac{K(Z)k_{rg}(s)dZ}{\mu[1 + \beta\Delta\sigma_{cr}(s) + \beta_a a]} \right] x \frac{\partial P}{\partial x} \quad (D4)$$

The total mobility in the three flow zones (0, 01, and 1) defined in Eq. (36) is given by the following relations:

i. Zone 0: comprising of the transition region and the brine region below it;

$$\Lambda_0(s) = \int_{Z_0}^1 \frac{K(Z)k_{rg}(s)dZ}{\mu[1 + \beta\Delta\sigma_{cr}(s) + \beta_a a]} + \int_0^{Z_0} K(Z)dZ \quad (D5)$$

ii. Zone 01: contains the mixed transition region between the injected gas (upper sub-zone) and displaced brine (lower sub-zone)

$$\Lambda_{01}(s) = \int_0^{Z_0} K(Z)dZ + \int_{Z_0}^{Z_0+h_c} k_{rw}(s)K(Z)dZ + \int_{Z_0}^{Z_0+h_c} \frac{K(Z)k_{rg}(s)dZ}{\mu[1 + \beta\Delta\sigma_{cr}(s) + \beta_a a]} + \frac{k_{rgwc}}{\mu[1 + \beta\Delta\sigma_{cr}(1) + \beta_a a]} \int_{Z_0+h_c}^1 K(Z)dZ \quad (D6)$$

iii. Zone 1: encompasses the transition region and the injected-gas plume beneath it

$$\Lambda_1(s) = \frac{k_{rgwc}}{\mu[1 + \beta\Delta\sigma_{cr}(1) + \beta_a a]} \int_{Z_0+h_c}^1 K(Z)dZ + \int_0^{Z_1} \left(k_{rw}(s)K(Z) + \frac{K(Z)k_{rg}(s)}{\mu[1 + \beta\Delta\sigma_{cr}(s) + \beta_a a]} \right) dZ \quad (D7)$$

Appendix E

Derivation of Injectivity and Sweep Efficiency

According to Eq. (35) the pressure drop at any given moment, τ is given by

$$\Delta P(\tau) = \int_{x_w}^{\infty} \left(-\frac{\partial P}{\partial x} \right) dx = \int_{x_w}^{\infty} \frac{1}{\Lambda(S)x} dx \quad (\text{E1})$$

For any given moment $\tau_i < \tau(D_0)$, three flow regions are present: the gas zone, the two-phase transition zone, and the brine zone ahead of the advancing front. The corresponding pressure drop at this moment is expressed as

$$\Delta P(\tau) = \int_{x_w}^{D_1\tau} \frac{1}{\Lambda(1)x} dx + \int_{D_1\tau}^{D_0\tau} \frac{1}{\Lambda(S)x} dx + \int_{D_0\tau}^{\infty} \frac{dP}{dx} dx = I_1 + I_2 + I_3 \quad (\text{E2})$$

In this expression, the first, second, and third integrals represent contributions from the gas zone, the transition zone, and the brine zone, respectively. Within the two-phase region, the pressure drop is reformulated using the self-similar variable ζ , where

$$d\zeta = F'(C_g) dC_g \quad (\text{E3})$$

Introducing the self-similar variable from Eq. (25) into the second integral of Eq. (E2) gives pressure drop within the two-phase zone as

$$I_2 = \int_{C_{g1}}^{C_{g0}} \frac{F'(C_g)}{F(C_g)\Lambda(C_g)} dC_g \quad (\text{E4})$$

For the low-compressible brine zone ahead of the advancing front, the pressure drop is obtained by applying the solution in Eq. (34) to the diffusivity equation (Eq. (31)), yielding

$$I_3 = \int_{D_0\tau}^{\infty} -\frac{dP}{dx} dx = \left[P_e - \frac{1}{\Lambda(0)} e^{(AD_0)} \text{Ei}(-AD_0) \right] - [P_e] = -\frac{1}{\Lambda(0)} e^{(AD_0)} \text{Ei}(-AD_0) \quad (\text{E5})$$

Substituting Eqs. (E4) and (E5) into Eq. (E2) results in an expression for the total pressure drop at time τ :

$$\Delta P(\tau) = \int_{x_w}^{D_1\tau} \frac{1}{\Lambda(1)x} dx + \int_{C_{g1}}^{C_{g0}} \frac{F'(C_g)}{F(C_g)\Lambda(C_g)} dC_g - \frac{1}{\Lambda(0)} e^{(AD_0)} \text{Ei}(-AD_0) \quad (\text{E6})$$

The well impedance, defined as the normalised reciprocal of the injectivity index, is expressed in terms of the pressure drop as

$$J_w(\tau) = \frac{II(\tau=0)}{II(\tau)} = \frac{Q(\tau=0)}{\Delta P(\tau=0)} \frac{\Delta P(\tau)}{Q(\tau)} \quad (\text{E7})$$

The ordinary differential equation in Eq. (24) admits a first integral that is useful for evaluating sweep efficiency. Integrating both sides of Eq. (24) over the domain $\mathcal{Q}$ in the plane (x, τ) bounded by the characteristics of velocities D_0 and D_1 and applying Green's theorem to compute the resulting double integral, yields

$$\iint \left[\frac{\partial C_g}{\partial \tau} + \frac{\partial F}{\partial x} \right] d\tau dx = \oint F d\tau - C_g dx = 0 \quad (\text{E8})$$

Because CO₂ concentration C_g remains constant along characteristics, the contour integral in Eq. (E8) reduced to

$$\overline{C_g}(\tau) = (1 - x_w)C_g\left(\frac{1}{\tau}\right) - \tau F\left(C_g\left(\frac{1}{\tau}\right)\right) + \tau \quad (\text{E9})$$

where the average CO₂ concentration is defined as

$$\overline{C_g}(\tau) = \int_{x_w}^1 C_g(x, \tau) dx \quad (\text{E10})$$

At early times, before the breakthrough of gas, $\left(0 < \tau < \frac{1}{D_0}\right)$, the average CO₂ concentration is

$$\overline{C_g}(\tau) = \tau \text{ with } C_g\left(\frac{1}{\tau}\right) = 0, \quad F\left(C_g\left(\frac{1}{\tau}\right)\right) = 0 \quad (\text{E11})$$

At intermediate times, $\left(\frac{1}{D_0} < \tau < \frac{1}{D_1}\right)$, the average CO₂ concentration becomes

$$\overline{C_g}(\tau) = (1 - x_w)C_g\left(\frac{1}{\tau}\right) - \tau F\left(C_g\left(\frac{1}{\tau}\right)\right) + \tau \quad (\text{E12})$$

At late times, once the system reaches a stable regime $\left(\frac{1}{D_1} < \tau < \infty\right)$, the average CO₂ concentration approaches $\overline{C_g}(\tau) = (1 - x_w)$ with $C_g\left(\frac{1}{\tau}\right) = 1$, $F\left(C_g\left(\frac{1}{\tau}\right)\right) = 1$