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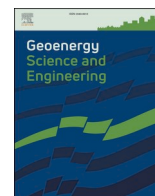
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Partly miscible CO₂-water displacement under vertical equilibrium with fines migration in layer-cake reservoirs

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ABSTRACT

Recent numerical simulations of geological CO₂ storage in deep saline aquifers have demonstrated that vertical equilibrium (VE) models provide a robust and computationally efficient approach for reservoir prediction and upscaling. These studies also underscore the significant impact of fines migration and partial water-CO₂ miscibility on the temporal evolution of storage behaviour. Specifically, capillary-driven detachment of clay and silica fines can reduce well injectivity, while water evaporation into the injected CO₂ causes near-wellbore drying, salt precipitation, and further injectivity impairment. However, current VE models do not capture these coupled physical and geochemical phenomena. For the first time, this work develops an extended VE model with the following novel features: (i) permeability-reducing migration of natural reservoir fines, (ii) water evaporation into injected CO₂, (iii) CO₂ dissolution into the displaced brine. For a stratified (layer-cake) aquifer, an exact analytical solution of the developed model has been derived. It provides explicit formulae for sweep efficiency and injectivity decline. The analytical model reveals two distinct displacement fronts – the displacement-dissolution front (advanced front) and the full evaporation front (receded front) – which bound the two-phase flow region. The model downscaling reveals that in formations with decreasing permeability with depth, gas saturation declines monotonically with depth. Alternatively, in reservoirs with increasing permeability with depth, the competition between viscous and gravitational forces can result in non-monotonic vertical saturation profiles. The analysis also shows that fines migration, while detrimental to injectivity, enhances sweep efficiency – highlighting a complex trade-off in the design and assessment of CO₂ storage operations.

Nomenclature

Latin letters

A	Inverse of pressure diffusivity coefficient, [L ⁻² T]
B	Power law exponent for straining, [-]
C	Averaged overall volumetric CO ₂ concentration, [-]
c	Microscale volumetric CO ₂ concentration, [-]
c_g	Volumetric fraction of CO ₂ dissolved in water, [-]
c_t	Total compressibility, [ML ⁻¹ T ⁻²]
c_w	Volumetric fraction of vaporised water in CO ₂ , [-]
f	Fractional flow of averaged gas saturation, [-]
f_0	Fractional flow of averaged gas saturation in zone 0, [-]
f_{01}	Fractional flow of averaged gas saturation in zone 01, [-]
f_1	Fractional flow of averaged gas saturation in zone 1, [-]
F	Overall fractional flow of averaged CO ₂ concentration, [-]
g	Gravitational acceleration, [LT ⁻²]
H	Reservoir thickness, [L]
H_c	Transition zone thickness, [L]

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h_c	Dimensionless thickness 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_T	Isothermal CO ₂ compressibility, [M ⁻¹ LT ²]
k_{rg}	Gas relative permeability, [-]
k_{rw}	Water relative permeability, [-]
k_{rgwi}	End point gas relative permeability, [-]
k_{rwgr}	End point water relative permeability, [-]
$<k>$	Average permeability, [L ²]

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(continued)

n_g	Corey fluid index for gas, [-]
n_w	Corey fluid index for water, [-]
p	Pressure, [ML ⁻¹ T ⁻²]
P	Dimensionless pressure, [-]
p_c	Capillary pressure [ML ⁻¹ T ⁻²]
p_d	Capillary pressure in water 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, [-]
p_{cr}	Critical pressure, [ML ⁻¹ T ⁻²]
$\langle p \rangle$	Average pressure, [ML ⁻¹ T ⁻²]
$\langle P \rangle$	Dimensionless average pressure, [ML ⁻¹ T ⁻²]
Q	Flow rate, [L ³ T ⁻¹]
r	Radial coordinate, [L]
r_e	Drainage radius, [L]
r_w	Well radius, [L]
S	Averaged gas saturation, [-]
s	Microscale gas saturation, [-]
S_0	Averaged gas saturation in zone 0, [-]
S_{01}	Averaged gas saturation in zone 01, [-]
S_1	Averaged gas saturation in zone 1, [-]
t	Time, [T]
T_{cr}	Critical temperature, [K]
U	Total flux, [LT ⁻¹]
U_g	Overall CO ₂ flux, [LT ⁻¹]
v_{gr}	Radial microscale gas flux, [LT ⁻¹]
v_{wr}	Radial microscale water flux, [LT ⁻¹]
V_{gr}	Averaged radial gas flux, [LT ⁻¹]
V_{wr}	Averaged radial water flux, [LT ⁻¹]
X	Dimensionless length, [-]
x_w	Dimensionless position of injection, [-]
z	Depth, [L]
Z	Dimensionless depth, [-]
z_0	Position of the advanced front, [L]
z_1	Position of the receded front, [L]
ΔP	Dimensionless pressure drop, [-]
Greek letters	
β	Formation damage coefficient, [-]
ε_c	capillary-viscous ratio; [-]
Φ	Porosity, [-]
μ	Gas-water viscosity ratio, [-]
μ_g	Gas viscosity, [ML ⁻¹ T ⁻¹]
μ_w	Water viscosity, [ML ⁻¹ T ⁻¹]
ρ^G	Density of pure CO ₂ component, [ML ⁻³]
ρ_g^W	Density of CO ₂ -rich gas phase (with dissolved water), [ML ⁻³]
ρ^W	Density of water component, [ML ⁻³]
ρ_w	Density of aqueous phase (with dissolved CO ₂), [ML ⁻³]
κ	Pressure-diffusivity coefficient, [L ² T ⁻¹]
ξ	Self-similar variable, [-]
σ_0	Initial detachable particle concentration, [-]
σ_{cr}	Maximum retention function, [-]
λ	Total mobility, [M ⁻¹ L ³ T]
λ_g	Gas mobility, [M ⁻¹ L ³ T]
λ_w	Water mobility, [M ⁻¹ L ³ T]
Λ	Dimensionless total mobility, [-]
ν	Relative range for permeability heterogeneity, [-]
η	Corey index for Leverett function, [-]
τ	Dimensionless time [-]
ω	Acentric factor, [-]
χ	Inverse function for downscaling, [-]

1. Introduction

Effective site screening for geological CO₂ storage, definition of optimal operational parameters, and reliable prediction of CO₂ plume migration relies heavily on the results of reservoir simulation. However, the inherent uncertainties in geological and hydrodynamic properties necessitate extensive sensitivity analyses through multi-variant model runs, rendering the simulation process computationally intensive and often impractically time-consuming. To address this challenge, current research efforts have focused on reducing the dimensionality of the flow problem. One promising approach is the use of vertical equilibrium (VE) models, which introduce VE pseudo-functions and corresponding upscaling techniques to simplify the simulation framework (Guo et al., 2014a, 2014b; Cowton et al., 2018; Nilsen et al., 2011, 2016; Alamara

et al., 2023a, 2023c; Andersen et al., 2015; Gray et al., 2012; Ahmadiania et al., 2019). The equations of VE model are derived from first principles (Coats et al., 1971; Zapata and Lake, 1981; Yortsos, 1992, 1995; Gray et al., 2012; Ahmadiania et al., 2019). VE models are deemed useful in supporting site selection for geological CO₂ storage, as well as in the planning and design of CO₂ storage projects in deep saline aquifers and depleted gas fields (Alamara et al., 2025a, 2025b). Conventional VE models are currently formulated for immiscible displacement only, i.e., interphase mass transfer is not accounted for (Bruining, 2021; Alamara et al., 2023b, 2025b). Variations of the VE immiscible model have been developed under different assumptions, particularly for gravity-dominated and capillary-dominated flow regimes. A representative, though incomplete, selection of the extensive literature on these topics includes the following references: (Alamara et al., 2023b; Eldoy et al., 1985; Zapata and Lake, 1981; Coats et al., 1967, 1971; Sorbie et al., 1994; Bear, 2013; Guo et al., 2016; Martin, 1958, 1968; Yortsos, 1992, 1995; Kurbanov, 1961; Fayers and Muggeridge, 1990).

The introduction of pseudo-functions in VE models transforms two-dimensional (x, z, t) or (r, z, t) flow problems into simplified one-dimensional (x, t) or (r, t) representations, allowing for explicit analytical solutions. These solutions can be readily used for rapid reservoir prediction and numerical grid upscaling. Moreover, VE models offer reliable substitutes for cumbersome inverse reservoir characterisation problem by analytical Welge or Johnson-Bossler-Naumann (JBN) methods (Bruining, 2021; Bedrikovetsky, 2013).

Evaporation of brine into the injected CO₂ and dissolution of CO₂ into the displaced brine can significantly influence the performance and dynamics of geological CO₂ storage (Russell and Bedrikovetsky, 2024; Aghajanian et al., 2024; Smith et al., 2025). The dissolution of CO₂ in formation brine leads to the formation of carbonic acid, which initiates a series of mineral dissolution and precipitation reactions that can alter reservoir properties. Concurrently, water evaporation into the CO₂ phase induces near-wellbore drying, triggering salt precipitation and consequent decline in well injectivity (Zhang et al., 2025). In contrast to fully segregated flow models, incorporating capillary pressure transforms the sharp water-gas interface into a capillary transition zone, which may extend beyond the reservoir thickness. Capillary forces acting on attached reservoir fines at the advancing water-gas menisci detaches and mobilizes these particles, resulting in fines migration with further straining in thin pores. This process causes permeability decline and further impairs injectivity, while also influencing overall sweep efficiency (Ge et al., 2022a, 2022b; Wang et al., 2022a, 2022b; Dalabayeva et al., 2025; Muneer et al., 2022a, 2022b, 2023). Despite the significance of these coupled processes, current VE models for CO₂-brine displacement remain limited to immiscible formulations and do not capture the effects of partial miscibility and fines migration.

Fig. 1 illustrates the schematic of radial water displacement by gas in a layer-cake reservoir, where permeability $k(z)$ decreases with depth. The mixed water-gas zone (in green) propagates behind the advancing front of formation brine. The gas saturation $s = 0$ at the water-gas front, denoted as $z = z_0(r, t)$, marks the leading edge of the displacement. The zone of dry, injected CO₂ (in yellow) follows the mixture flow zone, with gas saturation $s = 1$ at the evaporation front $z = z_1(r, t)$.

The reservoir fluid is two-phase binary mixture (Fig. 2a). Partial water-CO₂ miscibility is reflected by equilibrium concentrations of CO₂ dissolved in water, c_g , and water evaporated in the injected CO₂, c_w .

Fig. 3b depicts the case of a thin reservoir, where the capillary transition zone thickness exceeds the reservoir thickness, i.e., $z_1(r, t) - z_0(r, t) > H$. In contrast, Fig. 3a shows a thick reservoir, where the reservoir thickness exceeds that of the transition zone, $z_1(r, t) - z_0(r, t) < H$.

The vertical equilibrium (VE) model is valid when viscous pressure gradients are negligible compared to capillary and gravitational forces. In cases where the reservoir thickness significantly exceeds that of the capillary transition zone, the VE model simplifies to a segregated flow regime, with gas flowing above water in distinct layers (Bedrikovetsky,

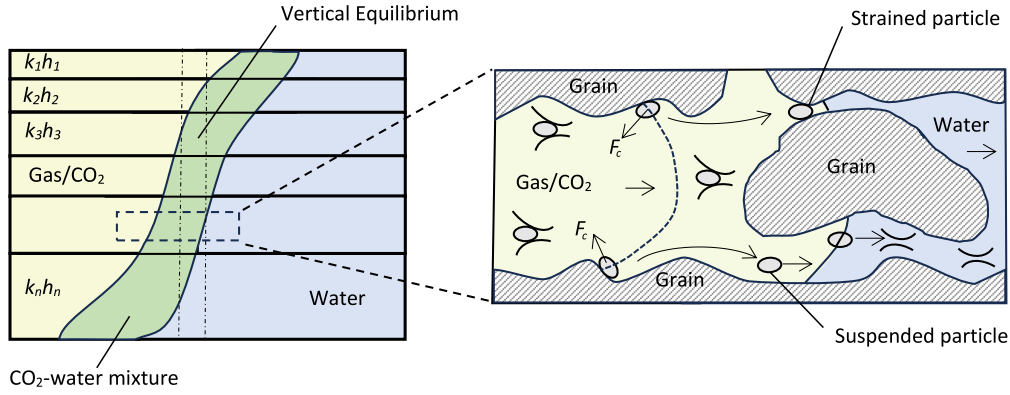


Fig. 1. Schematic for fines migration (fines detachment, migration and straining) under two-phase flow in porous media.

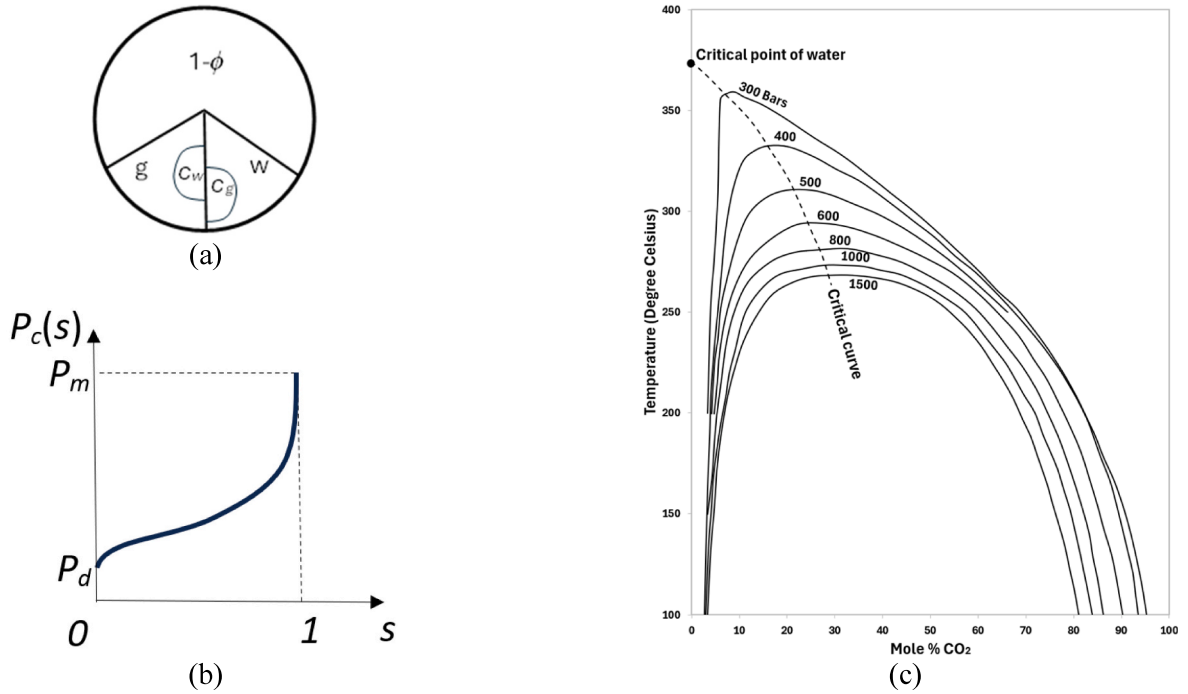


Fig. 2. Schematic for two phase binary mixture in porous media: (a) volumetric fractions of water and gas components in both phases; (b) capillary pressure curve as a function of gas saturation, s ; (c) isobaric curves in “gas fraction-temperature” phase diagram for binary water- CO_2 system.

2013). So, when the transition zone is much thicker than the reservoir, the system approaches a capillary-dominated two-phase flow scenario (Rabinovich et al., 2015, 2016). Under these conditions, assuming that the displacing phase fills the reservoir layers in order of decreasing permeability leads to the classical Dietz pseudo-functions (Bruining, 2021; Rabinovich et al., 2015, 2016; Cheng and Rabinovich, 2021; Dietz, 1953). However, in more general cases where viscous forces are non-negligible, this restrictive assumption no longer holds. More advanced flow models for viscous-dominated displacement waive the restrictive assumption of the filling of the layers by the displacing phase in order of permeability decrease (Yortsos, 1992, 1995; Hearn, 1971; Yuan and Shapiro, 2011).

We consider a water-wet porous medium, where capillary pressure increases with gas saturation s (Fig. 2b) ranging from the entry pressure p_d at full water saturation to a maximum value p_m where water saturation tends to zero. These capillary pressures – p_d and p_m – correspond to the advanced and receded displacement fronts, respectively, as shown in Fig. 3. Partial miscibility between water and CO_2 is represented by the mole fraction of CO_2 dissolved in water (c_g) and the mole fraction of

water evaporated into the injected CO_2 (c_w) (Fig. 2a). These quantities describe the mutual solubility of the two phases per unit pore volume and are functions of pressure and temperature under thermodynamic equilibrium conditions (Fig. 2c). At the pore scale, these mass transfer processes occur across capillary-controlled water-gas menisci, which advance through the pore space during displacement. Water evaporation into the injected CO_2 phase leads to salt precipitation from the brine, resulting in near wellbore plugging and a significant reduction in injectivity.

Current vertical equilibrium (VE) models for immiscible flow reduce the two-dimensional (2D) displacement problem to an exact Buckley-Leverett solution by using pseudo-functions to represent flow in an equivalent one-dimensional (1D) flow domain (Bruining, 2021). Similarly, the 1D two-phase displacement problem incorporating partial miscibility also admits an exact solution. Like the classical Buckley-Leverett formulation, this solution includes shock fronts and allows for graphical interpretation (Bedrikovetsky, 2013). Fig. 4a presents the phase diagram for a fixed pressure or temperature, corresponding to the thermodynamic conditions illustrated in Fig. 2c. The

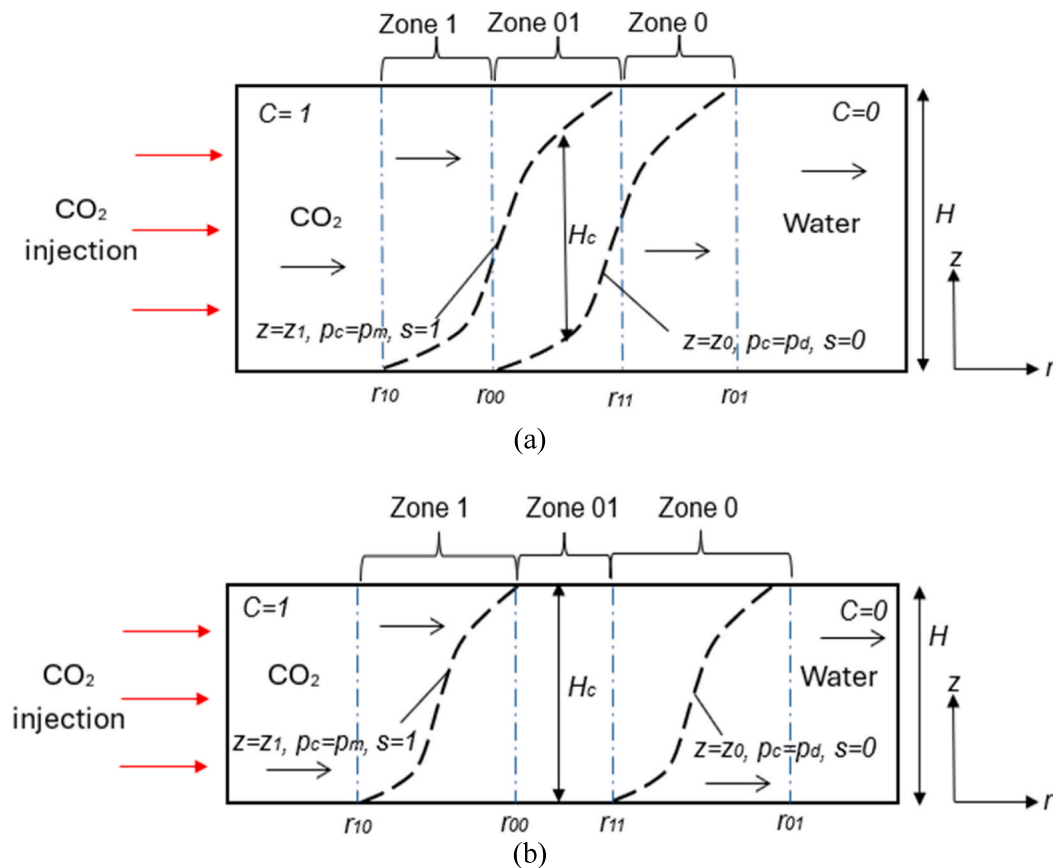


Fig. 3. Schematic for water displacement by CO₂ accounting for water evaporation and CO₂ dissolution in water: (a) in thick reservoir ($z_1(r, t) - z_0(r, t) < H$); (b) in thin reservoir ($z_1(r, t) - z_0(r, t) > H$).

flux of CO_2 in both phases depends on the overall CO_2 concentration, C , within the pore space. This functional relationship, $F(C)$, is shown as a continuous curve in Fig. 4b. The endpoints of the curve correspond to the displaced (pure water, $C = 0$) and injected (pure CO_2 , $C = 1$) states. The resulting concentration profile of CO_2 is shown in Fig. 4c. Starting from the injection point, the displacement domain consists of the following zones: (1) a dry CO_2 injection zone with $C = 1$; (2) a full evaporation front (transition from point 1 $\rightarrow$ 2); (3) a mixed-phase flow zone (2 $\rightarrow$ 3); (4) a water–gas front (transition from point 3 $\rightarrow$ 0); and (5) the flow zone of the undisturbed reservoir brine.

Fines migration is a well-documented phenomenon in CO₂ storage projects (Ge et al., 2022a, 2022b; Wang et al., 2022a, 2022b; Dalabayeve et al., 2025; Muneer et al., 2022a, 2022b, 2023). Naturally occurring reservoir fines, such as clays and silica particles, are typically adhered to rock surfaces and may be detached by drag, lift, or capillary forces. While these particles often form surface coatings and their detachment does not noticeably enhance permeability, their subsequent migration can lead to severe flow impairment. In particular, straining (size exclusion) of mobilized fines in narrow pore throats can drastically alter local flow dynamics, potentially causing a complete loss of permeability and hydraulic connectivity (Keykhosravi et al., 2025). Fig. 1 illustrates this process at the pore scale as a magnified view of the reservoir-scale system. Fines are detached by capillary forces and transported along advancing gas-water menisci, ultimately becoming trapped in constricted pores. Displacement proceeds in a piston-like fashion, with sequential meniscus positions indicated by dashed and solid lines. Residual, capillary-trapped water in micro-pores is omitted for clarity. Strained or re-attached fines remain within the gas-occupied

pore space, reducing permeability to the displacing CO₂ phase while having negligible effect on the already displaced water.

Despite the significant impact of fines migration, partial CO₂-water miscibility, and capillary pressure on CO₂ injection into saline aquifers, existing vertical equilibrium (VE) models do not incorporate these coupled physical processes. The present study addresses this gap by developing an extended VE framework that accounts for these critical phenomena.

In this paper, a new quasi-2D governing system for gas–water flow under vertical equilibrium (VE) conditions, accounting for mutual CO₂–water miscibility and fines migration, is derived. We average the quasi-2D system yielding its reduction to 1D hyperbolic conservation law and found an exact self-similar solution for the displacement of water by CO₂. The solution yields new explicit formulae for phase saturations, component concentrations, and reservoir pressure. To match the pressure distribution in the incompressible region behind the displacement front with the initial reservoir pressure, a small compressibility is introduced ahead of the displacement front. The VE assumption enables downscaling of the analytical 1D solution in radial–temporal coordinates (r, t) to reconstruct full vertical distributions (r, z, t) of saturation, concentration, and pressure. The downscaling procedure has been formulated. The downscaled profiles reveal novel phenomena of saturation profile monotonicity depending on whether permeability increases or decreases with depth: in formations where permeability decreases with depth, gas saturation decreases monotonically with depth, while in formations with increasing permeability with depth, the competition between viscous and gravitational forces may produce non-monotonic vertical saturation profiles. It was found that fines migration

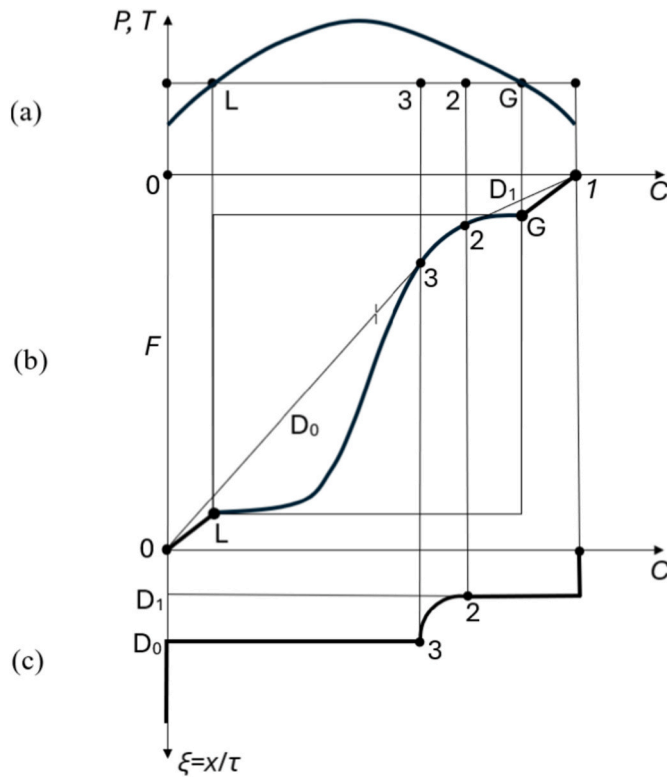


Fig. 4. Form of fractional flow that accounts for partial miscibility between water and CO₂: (a) phase diagram for pressure/temperature versus overall CO₂ concentration in gaseous and aqueous phases; (b) fractional flow versus CO₂ concentration; (c) overall CO₂ concentration in both phases versus ξ

and the resulting permeability reduction led to a decline in well injectivity, while enhancing reservoir sweep and increasing overall CO₂ storage capacity.

The structure of the manuscript is as follows. Section 1 introduces the key physical phenomena influencing water displacement by CO₂, which are incorporated into the proposed model. Section 2 outlines the model assumptions and derives the governing equations for both incompressible and compressible zones. Section 3 presents vertically averaged “pseudo-function” model and pressure diffusivity equation in the displaced-brine-flow zone. Section 4 derives the self-similar solution to the averaged model and analytical formulae for pressure in the low compressible undisturbed zone as well as total mobility. Section 5 presents explicit formulae for well injectivity and sweep efficiency calculations including the procedure for practical engineering calculations. Section 6 details the downscaling procedure used to reconstruct full vertical profiles from the 1D solution. Section 7 conducts a sensitivity analysis with respect to reservoir properties and injectivity parameters. Sections 8 and 9 provide a discussion of results and concluding remarks.

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

This section presents the main assumptions of VE model for displacement in layer-cake reservoir accounting for partial CO₂-brine miscibility and fines migration (section 2.1) and schematic for flow zone structure (section 2.2).

2.1. Assumptions and formulation of 2D model

We assume incompressibility of CO₂. Appendix A proves negligible increase of supercritical CO₂ density from the reservoir top to the

bottom, comparing with the averaged density value. Besides, for the cases where pressure drawdown during CO₂ injection is significantly lower than the average reservoir pressure, the reservoir pressure is constant, and CO₂ density variation over the reservoir is significantly lower than the averaged density. For low injection rates and the reservoir pressures and temperatures where Joule-Thomson cooling is negligible, the temperature can also be assumed constant (Chesnokov et al., 2025).

We consider binary two-phase water-CO₂ mixture as a reservoir fluid. By Gibbs’ rule, it has two degrees of freedom (2-2+2), so CO₂ concentration in water c_w and vapor concentration in injected CO₂ c_g are functions of pressure and temperature. In the case where reservoir pressure and temperature are constant, concentrations c_w and c_g are constant.

We discuss radial injection into layer cake reservoir with hydraulically connected horizontal layers: $k = k(z)$. The reservoir is assumed radially homogeneous, i.e. the lateral heterogeneity is neglected. The reservoir thickness H is assumed to be constant. The brine salinity is assumed constant.

Flow zones with water-gas mixture – The aqueous and gaseous phases are assumed to contain water and CO₂ components. The mixing of these components is described using Amagat’s law of additive volumes, under the assumption that the individual densities of CO₂ and water remain constant and equal in both phases. This allows for the introduction of volumetric concentrations for each component in the respective phases.

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

where ρ^G and ρ^W correspond to densities of pure components (CO₂ and water, respectively), while ρ_g and ρ_w are phase densities (CO₂-rich fluid with vaporised water and water-rich fluid with dissolved CO₂, respectively). Pressures and temperatures are constant. Phase equilibrium is assumed, so c_w and c_g are also constant, representing the fraction of water vaporised into gas and the fraction of gas dissolved in water, respectively, as shown in Fig. 2a. The overall volumetric CO₂ concentration in both phases and the overall CO₂ flux consisting of those in both phases are given, respectively, as,

$$c = (1 - c_w)s + c_g(1 - s), u_{gr} = (1 - c_w)v_{gr} + c_g v_{wr}, \quad (2)$$

Hydrostatic pressure is assumed for each phase, i.e.

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

The rock remains water-wet during the overall displacement, so $p_g > p_w$:

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

where the capillary pressure p_c is expressed via dimensionless Leverett function $J(s)$

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

The model accounts for formation damage induced by fines migration. It is assumed that at the reservoir scale, fines detachment, migration and straining occur instantly if compared with the time in one Pore-Volume-Injected (PVI). The detaching capillary force, exerting on the attached particle, is significantly higher than the attaching electrostatic force. So, all detachable fines are detached by the advanced gas-water menisci during passing via a pore. Therefore, the concentration of attached fines in the rock is a function of saturation - $\sigma_{cr}(s)$ (Russell et al., 2025; Nguyen et al., 2022). It is called the maximum retention function (MRF). Lab tests show that MRF can be approximated by power-law dependency with high accuracy (Nguyen et al., 2022)

$$\sigma_{cr}(s) = \sigma_0 (1 - s)^B \quad (6)$$

where the power law exponent for straining B and overall concentration of detachable fines σ_0 are empirical constants, that characterise the retention behaviour. The concentration of strained fines at saturation s is equal to the difference of the initial attached fines concentration and the maximum retained concentrations:

$$\Delta\sigma_{cr} = \sigma_{cr}(0) - \sigma_{cr}(s) \quad (7)$$

Modification to Darcy's law for two-phases gives the expressions for phase velocities accounting for the formation damage factor in the gas phase only where β is the formation damage coefficient.

$$v_{wr} = -\frac{k(z)k_{rw}(s)}{\mu_w} \frac{\partial p_w}{\partial r}, v_{gr} = -\frac{k(z)k_{rg}(s)}{\mu_g[1 + \beta\Delta\sigma_{cr}(s)]} \frac{\partial p_g}{\partial r} \quad (8)$$

The schematic in Fig. 1 illustrates the behaviour of detached fines that migrate through the porous medium, transported by the detaching meniscus, until they are retained by straining. As shown, a migrating particle may become trapped within a narrow pore throat, effectively plugging the pore. Once straining occurs, the ensemble of menisci continues to advance beyond the obstructed region. Consequently, the presence of strained particles results in a reduction of permeability within the flow domain of the displacing phase, while the displaced phase remains unaffected. Therefore, in Eq. (8), the damage is expressed exclusively for the gas phase.

Undisturbed zone of displaced reservoir fluid flow – In the single-phase zone containing the displaced reservoir fluid, $s = 0$, the hydrostatic pressure distribution is described by the second equation in Eq. (3). In this region, both the reservoir brine and the rock matrix are assumed to exhibit low compressibility, i.e.,

$$\phi(p)\rho_w(p) = \phi_0\rho_{w0} \exp\left[-\frac{p-p_0}{c_t}\right] \quad (9)$$

where index “0” corresponds to “initial conditions”, and c_t is the total compressibility coefficient for fluid and rock (Dake, 1983).

Dry zone of the displacing fluid flow – Here, $s = 1$, and the depth hydrostatic pressure distribution is assumed too. Yet, the displacing gas is assumed to be incompressible. Index “1” corresponds to the gas zone in Fig. 3a b.

2.2. Water-gas and evaporation fronts in 2D displacement model

Fig. 3 illustrates the schematic of water displacement by CO₂ in a layer-cake reservoir. Ahead of the displacement front, at $z < z_0(r, t)$, no CO₂ is present; thus, the gas saturation is $s = 0$ and the CO₂ concentration is $c_g = 0$ in this region. The model accounts for water evaporation into injected CO₂ assuming that the reference time of evaporation is significantly lower than the injection time of 1 PVI. Indeed, for drainage radius $r_e = 500$ m and core length $L = 0.05$ m, 1 PVI of the reservoir corresponds to $(500/0.05)^2 = 10^8$ PVIs of the core. Keykhosravi et al. (2025) and Russell and Bedrikovetsky (2024) present full evaporation time as 10^4 - 10^5 PVIs, which is negligibly smaller than 1 PVI time, supporting the hypothesis of instant evaporation at the reservoir scale. So, at the reservoir scale, phase concentrations c_w and c_g are established instantly. Behind the rear front of complete evaporation, at $z > z_1(r, t)$, no water remains, resulting in zone $s = 1$ and $c_g = 1$. Therefore, the saturation is $s = 0$ ahead of the displacement front and $s = 1$ behind the rear front. Saturation continuously increases from zero to one across the mixture zone.

3. Derivation of the averaged “pseudo-function” model

This section derives the averaged flow equation – VE model – including development of the fractional flow expressions (section 3.1),

derivation of volumetric balance equations (section 3.2), and obtaining the solution for pressure in the flow zone of low-compressible fluid (section 3.3).

3.1. Expressions for fractional flows

The difference of the hydrostatic pressures given by Eq. (3) yields the first order derivative for capillary pressure as

$$\frac{dp_c}{dz} = \Delta\rho g, \Delta\rho = \rho_w - \rho_g \quad (10)$$

The gas saturation and capillary pressure at the advanced front, z_0 and the receded front, z_1 are given as:

$$z = z_0(r, t) : s = 0, p_c = p_d \quad (11)$$

$$z = z_1(r, t) : s = 1, p_c = p_m \quad (12)$$

Taking the integral of Eq. (10) yields

$$p_c = \Delta\rho g z + \text{const} \quad (13)$$

Substituting Eqs. 11 and 12 into Eq. (13) and taking the difference of the resulting equations yields the expression for the thickness of the capillary transition zone, H_c .

$$p_m - p_d = \Delta\rho g H_c, H_c = z_1(r, t) - z_0(r, t) \quad (14)$$

Here we assume common Leverett function for all layers, so the threshold and maximum capillary pressures, p_d and p_m , depend on porous media

$$p_d = \frac{\sigma \cos \theta}{\sqrt{k(z)/\phi}} J_d, p_m = \frac{\sigma \cos \theta}{\sqrt{k(z)/\phi}} J_m, \quad (15)$$

where J_d and J_m are constant representing the values of the Leverett J function at $s = 0$ and $s = 1$, respectively, as

$$J_d = J(0), J_m = J(1) \quad (16)$$

Substitution of Eq. (15) into Eq. (14) yields

$$\sigma \cos \theta \sqrt{\phi} \left(\frac{J_m}{\sqrt{k(z_1(r, t))/\phi}} - \frac{J_d}{\sqrt{k(z_0(r, t))/\phi}} \right) = \Delta\rho g H_c \quad (17)$$

exhibiting r - and t -dependence of the transition zone thickness.

Thick Reservoirs ($z_1(r, t) - z_0(r, t) < H$), Fig. 3a – We now derive averaged equations for the case of thick reservoirs, where the reservoir thickness, H , exceeds the thickness of the transition zone, H_c .

Taking the integral of Eq. (10) from z to z_0 accounting for Eq. (11) yields the expression for capillary pressure at the advanced front as

$$p_c(s, z) - p_d = \Delta\rho g \cdot (z - z_0) = \frac{\sigma[J(s) - J_d]}{\sqrt{k(z)/\phi}}, J(s) = J_d + (z - z_0) \frac{\Delta\rho g}{\sigma} \sqrt{k(z)/\phi} \quad (18)$$

Considering the inverse function to Eq. (18), $j = J^{-1}$, the vertical saturation distribution is obtained as

$$s = j \left(J_d + (z - z_0) \frac{\Delta\rho g}{\sigma} \sqrt{k(z)/\phi} \right) \quad (19)$$

Here we consider only s -dependency of Leverett function, which is a common assumption (Bruining, 2021). For power-law $J(s)$, inverse function j in Eq. (19) is also expressed as power-law. In a general case of $J(s, z)$, saturation s in Eq. (19) is a root of transcendental Eq. (18).

Substituting Eq. (19) into the first equation of Eq. (2) gives gas

concentration in two-phase zone at $z = z_0$ as

$$c = j \left(J_d + (z - z_0) \frac{\Delta \rho g}{\sigma} \sqrt{k(z)/\phi} \right) (1 - c_w - c_g) + c_g \quad (20)$$

Similarly, taking the integral of Eq. (10) from z to z_1 accounting for Eq. (12) yields the expression for capillary pressure at the receded front as

$$p_c(s, z) - p_m = \Delta \rho g \cdot (z - z_1) = \frac{\sigma [J(s) - J_m]}{\sqrt{k(z)/\phi}}, J(s) = J_m + (z - z_1) \frac{\Delta \rho g}{\sigma} \sqrt{k(z)/\phi} \quad (21)$$

Substituting the inverse function of Eq. (21), $j = J^{-1}$ into Eq. (2) gives the gas concentration in two-phase zone at $z = z_1$ as

$$c = j \left(J_m + (z - z_1) \frac{\Delta \rho g}{\sigma} \sqrt{k(z)/\phi} \right) (1 - c_w - c_g) + c_g \quad (22)$$

The average gas saturation across the reservoir thickness, S , and average CO₂ concentration, C , are determined by the expressions

$$S(r, t) = \frac{1}{H} \int_0^H s(r, z, t) dz, C = S(1 - c_w) + (1 - S)c_g \quad (23)$$

where zones 0, 01 and 1 represent the regions with “mixture above water”, “mixture between gas and water” and “mixture below gas” respectively as illustrated in Fig. 3a, b, ie.,

$$0 : r_{11} < r < r_{01}, 01 : r_{00} < r < r_{11}, 1 : r_{10} < r < r_{00} \quad (24)$$

As it follows from Eq. (3), pressure gradients are independent of z . Therefore, with averaging of phase velocities over z in Eq. (8), pressure gradients are taken out of the integrals, Eq. (B1). This allows defining upscaled (pseudo functions) phase permeabilities as functions of either average saturation S or positions of fronts z_0 or z_1 .

The fractional flow of gaseous phase is defined in terms of the phase mobilities, expressed in Eq. (B8):

$$f = \frac{\int_0^H \frac{k(z)k_{rg}(s)dz}{\mu_g[1 + \beta\Delta\sigma_{cr}(s)]}}{\left[\int_0^H \frac{k(z)k_{rw}(s)dz}{\mu_w} + \int_0^H \frac{k(z)k_{rg}(s)dz}{\mu_g[1 + \beta\Delta\sigma_{cr}(s)]} \right]} = \frac{\lambda_g(S)}{[\lambda_w(S) + \lambda_g(S)]} = \frac{\lambda_g(S)}{\lambda(S)}, \quad (25)$$

where the overall fractional flow of CO₂ component is expressed in terms of Eq. (25) as

$$F = (1 - c_w)f + (1 - f)c_g \quad (26)$$

From Eq. (B6), the overall gas flux (detailed derivation is provided in Appendix B) in terms of the overall fractional flow of CO₂ (Eq. (26)) becomes

$$U_g = UF + [F - (1 - c_w)] \int_0^H \frac{k(z)k_{rg}(s)dz}{\mu_g[1 + \beta\Delta\sigma_{cr}(s)]} \frac{\partial p_c}{\partial r} \quad (27)$$

Calculations of the averaged overall CO₂ concentration C and fractional flow F in thick reservoir are presented in Table 1. The equations for averaged gas saturation S_0 , CO₂ concentration C_0 and fractional flow for averaged gas saturation $f_0(S)$ for the zone 0 - “mixture above water” are given in second line of Table 1. Third line of Table 1 contains those three expressions for the zone 01 - “mixture between gas and water”. The formulae for zone 1 - “mixture below gas” are presented in fourth line. Overall fractional flows for CO₂-component $F_0(C)$, $F_{01}(C)$, and $F_1(C)$ are obtained using Eq. (26).

Thin Reservoirs ($z_1(r, t) - z_0(r, t) > H$), Fig. 3b – For the case of thin reservoirs, where the capillary transition zone is thicker than the reservoir, the expression for capillary pressure, vertical saturation distribution, the gas concentration in two-phase zone at the advanced front and receded front ($z_0(r, t)$ and $z_1(r, t)$, respectively) are the same as those derived for thick reservoir given by Eqs 18, 19, 20, 21, and 22. Table 2 contains the equations for overall gas saturation $S(r, t)$ (column two), CO₂ concentration (column 3), and fractional flow for gas phase $f(S)$ (column four). The second row of Table 2 presents those formulae for zone 0 - “mixture above water”. Those expressions for the zone 01

Table 1
Expressions for averaged gas component concentration and fractional flux in different regions of thick reservoir.

Zone	$S(r, t)$	Averaged overall CO ₂ concentration $C = S(1 - c_w) + (1 - S)c_g$	Fractional flow of averaged gas saturation $f(S)$
0	$\frac{1}{H} \int_{z_0}^H \left(J_d + (z - z_0) \frac{\Delta \rho g}{\sigma} \sqrt{k(z)/\phi} \right) dz$	$c_g + \frac{(1 - c_w - c_g)}{H} \int_{z_0}^H \left(J_d + (z - z_0) \frac{\Delta \rho g}{\sigma} \sqrt{k(z)/\phi} \right) dz$	$\frac{\int_{z_0}^H \frac{k(z)k_{rg}(s)dz}{[1 + \beta\Delta\sigma_{cr}(s)]}}{\left[\frac{\mu_g}{\mu_w} \int_0^{z_0} k(z)k_{rw}(0)dz + \int_{z_0}^H \frac{k(z)k_{rg}(s)dz}{[1 + \beta\Delta\sigma_{cr}(s)]} \right]}$
01	$\frac{1}{H} \int_{z_0}^{z_0+H_c} s(r, z, t) dz + \frac{(H - H_c - z_0)}{H}$	$c_g + (1 - c_w - c_g) \cdot \left[\frac{1}{H} \int_{z_0}^{z_0+H_c} s(r, z, t) dz + \frac{(H - H_c - z_0)}{H} \right]$	$\left[\int_{z_0}^{z_0+H_c} \frac{k(z)k_{rg}(s)dz}{[1 + \beta\Delta\sigma_{cr}(s)]} + \frac{k_{rgwc}}{[1 + \beta\Delta\sigma_{cr}(1)]} \int_{z_0+H_c}^H k(z)dz \right] \cdot \left\{ \frac{\mu_g}{\mu_w} \left(\int_0^{z_0} k(z)k_{rw}(0)dz + \int_{z_0}^{z_0+H_c} \frac{k(z)k_{rw}(s)dz}{\mu_w} \right) + \int_{z_0+H_c}^H \frac{k(z)k_{rg}(s)dz}{[1 + \beta\Delta\sigma_{cr}(s)]} + \frac{k_{rgwc}}{[1 + \beta\Delta\sigma_{cr}(1)]} \int_{z_0+H_c}^H k(z)dz \right\}^{-1}$
1	$\frac{1}{H} \int_0^{z_1} \left(J_m + (z - z_1) \frac{\Delta \rho g}{\sigma} \sqrt{k(z)/\phi} \right) dz + \frac{(H - z_1)}{H}$	$c_g + (1 - c_w - c_g) \cdot \left\{ \frac{1}{H} \int_0^{z_1} \left(J_m + (z - z_1) \frac{\Delta \rho g}{\sigma} \sqrt{k(z)/\phi} \right) dz + \frac{(H - z_1)}{H} \right\}$	$\left[\int_0^{z_1} \frac{k(z)k_{rg}(s)dz}{[1 + \beta\Delta\sigma_{cr}(s)]} + \frac{k_{rgwc}}{[1 + \beta\Delta\sigma_{cr}(1)]} \int_{z_1}^H k(z)dz \right] \cdot \left\{ \frac{\mu_g}{\mu_w} \int_0^{z_1} k(z)k_{rw}(s)dz + \int_0^{z_1} \frac{k(z)k_{rg}(s)dz}{[1 + \beta\Delta\sigma_{cr}(s)]} + \frac{k_{rgwc}}{[1 + \beta\Delta\sigma_{cr}(1)]} \int_{z_1}^H k(z)dz \right\}^{-1}$

Table 2

Expressions for averaged gas component concentration and fractional flux in different regions of thin reservoir.

Zone	$S(r, t)$	Averaged overall CO ₂ concentration $C = S(1 - c_w) + (1 - S)c_g$	Fractional flow for averaged gas saturation $f(S)$
0	$\frac{1}{H} \int_{z_0}^H j_0 \left(J_d + (z - z_0) \frac{\Delta \rho g}{\sigma} \sqrt{k(z)/\phi} \right) dz$	$c_g + \frac{(1 - c_w - c_g)}{H} \int_{z_0}^H j_0 \left(J_d + (z - z_0) \frac{\Delta \rho g}{\sigma} \sqrt{k(z)/\phi} \right) dz$	$\frac{\int_{z_0}^H \frac{k(z)k_{rg}(s)dz}{[1 + \beta\Delta\sigma_{cr}(s)]}}{\left[\frac{\mu_g}{\mu_w} \int_0^{z_0} k(z)k_{rw}(0)dz + \int_{z_0}^H \frac{k(z)k_{rg}(s)dz}{[1 + \beta\Delta\sigma_{cr}(s)]} \right]}$
01	$\frac{1}{H} \int_0^H s(r, z, t) dz$	$c_g + (1 - c_w - c_g) \frac{1}{H} \int_0^H s(r, z, t) dz$	$\frac{\int_0^H \frac{k(z)k_{rg}(s)dz}{[1 + \beta\Delta\sigma_{cr}(s)]}}{\left[\frac{\mu_g}{\mu_w} \int_0^H k(z)k_{rw}(s)dz + \int_0^H \frac{k(z)k_{rg}(s)dz}{[1 + \beta\Delta\sigma_{cr}(s)]} \right]}$
1	$\frac{1}{H} \int_0^{z_1} j_1 \left(J_m + (z - z_1) \frac{\Delta \rho g}{\sigma} \sqrt{k(z)/\phi} \right) dz + \frac{(H - z_1)}{H}$	$c_g + (1 - c_w - c_g) \cdot \left\{ \frac{1}{H} \int_0^{z_1} j_1 \left(J_m + (z - z_1) \frac{\Delta \rho g}{\sigma} \sqrt{k(z)/\phi} \right) dz + \frac{(H - z_1)}{H} \right\}$	$\left[\int_0^{z_1} \frac{k(z)k_{rg}(s)dz}{[1 + \beta\Delta\sigma_{cr}(s)]} + \frac{k_{rgwc}}{[1 + \beta\Delta\sigma_{cr}(1)]} \int_{z_1}^H k(z)dz \right] \cdot \left\{ \frac{\mu_g}{\mu_w} \int_0^{z_1} k(z)k_{rw}(s)dz + \int_0^{z_1} \frac{k(z)k_{rg}(s)dz}{[1 + \beta\Delta\sigma_{cr}(s)]} + \frac{k_{rgwc}}{[1 + \beta\Delta\sigma_{cr}]} \int_{z_1}^H k(z)dz \right\}^{-1}$

“mixture between gas and water” are given in the third row of [Table 2](#). The fourth row of [Table 2](#) corresponds to zone 1 - “mixture below gas”. The overall fractional flow of CO₂-component versus its concentration F (C) is calculated using Eq. (26).

3.2. 1D averaged mass balance for gas

The equation for 1D two-phase flow of partly miscible fluids in heterogeneous non-deformable porous media follows from substituting the dimensionless variables and parameters Eq. (B3) into Eq. (C2) to obtain:

$$\frac{\partial C}{\partial \tau} + \frac{\partial F}{\partial x} = -\varepsilon_c \frac{\partial}{\partial x} \left[(F - (1 - c_w)) \int_0^1 \frac{K(Z)k_{rg}(s)dZ}{\mu(1 + \beta\Delta\sigma_{cr}(s))} x \frac{\partial J(s)}{\partial x} \right] \quad (28)$$

where ε_c is the capillary-viscous ratio; the expressions for overall fractional flow of CO₂ are presented in [Tables 1 and 2](#).

Large scale approximation corresponds to negligibly small value of capillary-viscous ratio where

$$\varepsilon_c = \frac{4\pi k_0 H}{Q\mu_w} \frac{\sigma \cos \theta \sqrt{\phi}}{\sqrt{k_0}} \ll 1 \quad (29)$$

Considering the following typical values for interfacial tension, $\sigma = 20$ mN/m; contact angle, $\theta = 30^\circ$; reservoir thickness, $H = 15$ m; average absolute permeability, $k_0 = 3.5 \times 10^{-13}$ m²; viscosity of water, $\mu_w = 1.0$ mPa·s and injection rate, $Q = 1.3 \times 10^{-2}$ m³/s, the value of $\varepsilon_c \approx 0.08 \ll 1$ ([Dake, 1983](#)).

For large scale approximations, the mass balance equation Eq. (28) yields a hyperbolic equation given as

$$\frac{\partial C}{\partial \tau} + \frac{\partial F(C)}{\partial x} = 0 \quad (30)$$

An initial-boundary value problem for Eq (30), describing displacement of water by CO₂ is formulated as follows:

$$\begin{cases} t = 0 : C = 0 \\ r = r_w : C = 1 \end{cases} \quad (31)$$

Substitution of the dimensionless parameters Eq. (B3) expresses the initial-boundary value problem as

$$\begin{cases} \tau = 0 : C = 0 \\ x = x_w = \left(\frac{r_w}{r_e} \right)^2 : C = 1 \end{cases} \quad (32)$$

3.3. Pressure diffusivity equation in undisturbed zone

Under the assumptions of hydrostatic pressure distribution and low compressibility of water and rock, [Appendix C](#) derives the pressure diffusivity equation

$$\frac{\partial \langle P \rangle}{\partial \tau} = \kappa \frac{\partial}{\partial x} \left(x \frac{\partial \langle P \rangle}{\partial x} \right) \quad (33)$$

where $\langle P \rangle$ is the averaged over depth reservoir pressure, κ is the pressure-diffusivity coefficient that corresponds to averaged permeability, introduced in Eq. (D5).

4. Large-scale analytical model

This section derives the analytical model – solution for averaged VE equations – that includes the expressions for saturations and concentrations in the incompressible flow zone (section 4.1), the solution in the compressible flow zone (section 4.2), and the expression for total two-phase mobility (section 4.3).

4.1. Buckley–Leverett solution for concentrations and saturation

Let us derive exact solution of initial-boundary problem (30) for Eq. (32). Applying the chain rule to the second term of Eq. (30) yields

$$\frac{\partial C}{\partial \tau} + \frac{dF}{dC} \frac{\partial C}{\partial x} = 0 \quad (34)$$

Introducing the self-similar variable, $\xi = x/\tau$,

$$C(x, \tau) = \tilde{C}(\xi), \xi = x/\tau \quad (35)$$

The solution to the initial-boundary value problem Eqs. 30 and 32 is

$$C(\xi) = \begin{cases} 1, & \frac{x_w}{\tau} < \xi < D_1 \\ \xi = \frac{x}{\tau} = F(C), & D_1 < \xi < D_0 \\ 0, & D_0 < \xi < \infty \end{cases} \quad (36)$$

Mass balance (Hugoniot-Rankine) conditions are fulfilled on the shock fronts Z_0 and Z_1 . The shock velocities at the advanced and receded front are

$$\begin{aligned} \frac{dx}{d\tau}(Z_0) &= D_0 = \frac{F(C^+) - F(C^-)}{C^+ - C^-} = \frac{F(C^-)}{C^-}, \quad \frac{dx}{d\tau}(Z_1) = D_1 \\ &= \frac{F(C^+) - F(C^-)}{C^+ - C^-} = \frac{F(C^+) - 1}{C^+ - 1} \end{aligned} \quad (37)$$

Fig. 4a-c illustrates a typical form of fractional flow curve obtained for a binary mixture of water and CO₂ that accounts for partial miscibility between water and CO₂, and the nature of the self-similar solution in terms of ξ .

The results of reservoir behaviour prediction based on exact solution (36, 37) are shown in Fig. 5 for five values of viscosity ratio. Here we consider layer-cake reservoir with $k(z)$ given by third-order polynomial

$$k(z) = (k_{\max} - k_{\min})\left(\frac{z}{H}\right)^3 + k_{\min} \rightarrow k(Z) = (k_{\max} - k_{\min})Z^3 + k_{\min} \quad (38)$$

The minimum and maximum permeabilities are $k_{\min} = 2mD$, $k_{\max} = 700mD$. In this study, we consider a base case for the reservoir of thickness, $H = 25m$ with reservoir pressure of $p_e = 400$ bars and temperature of $120^\circ C$. As it follows from phase diagram in Fig. 2b, $c_g = 0.03$, $c_w = 0.09$. The Leverett function for capillary pressure and Corey relative permeability are expressed as:

$$J(s) = C(s)^{-\eta}, \quad k_{rg}(s) = k_{rgwi}(s)^{n_g}, \quad k_{rw}(s) = k_{rwgr}(1 - s)^{n_w} \quad (39)$$

where the Corey index, $\eta = 1.3$; the end point saturations of gas and water are 0 and 0.2, respectively; the end point relative permeability of gas and water are $k_{rgwi} = 0.6$ and $k_{rwgr} = 1$. The fluid exponents for gas and water are $n_g = 3$ and $n_w = 5$. The following typical values are used to describe formation damage due to fines migration, Eq. (6): power law exponent for straining, $B = 1.73$; total detachable fines concentration on the rock surface, $\sigma_0 = 7.12 \times 10^{-4}$; the formation damage coefficient, $\beta = 1.5 \times 10^4$.

Fig. 5a presents the plot of fractional flow function $F(C)$ for a viscosity ratio of $\mu = \mu_g/\mu_w = 0.021$ (blue curve). The plot consists of three distinct regions: a straight-line connecting point 1 and G, representing

undersaturated single-phase gas flow; an S-shaped curve between points G and L, corresponding to the two-phase flow region; and a straight-line from point O to L, denoting undersaturated single-phase water flow as illustrated in Fig. 4b. The slopes of both straight-line segments are unity, indicating that, in the single-phase regions, each component is transported entirely by the total flux of the respective carrier phase. Notably, the fractional flow functions in the single-phase regions are independent of phase viscosities.

Fig. 5b shows the corresponding breakthrough gas-cuts $F(C)$ versus PVI at $x = 1$. Blue curve is the breakthrough CO₂-cut, which is the CO₂-flux in both phases. After fast breakthrough of low-viscosity gas (at 0.2PVI), gas-cut jumps up to 0.65 and then quickly increasing until 0.9 at the moment of 6.4 PVI. Then gas-cut jumps at this moment to 1. Beyond this moment of long-term injection, the stabilization and complete evaporation of water into the injected CO₂ occurs.

4.2. Pressure distribution in the reservoir

Let us derive an analytical model for the low-compressible flow ahead of the displacement front. Below we show that 2D single-phase low-compressible flow can be averaged in z , yielding traditional 1D pressure-diffusivity equation. The 2D mass balance equation for low-compressible water ahead of the advanced front is

$$\frac{\partial}{\partial t}(\phi \rho_w) + \frac{1}{r} \frac{\partial}{\partial r}(\tau \rho_w u_{wr}) + \frac{\partial}{\partial z}(\rho_w u_{wz}) = 0 \quad (40)$$

It is assumed that the rate at the advanced front is equal to the injection rate and the pressure at a location far from the injection well is equal to the reservoir pressure. Hence, the following boundary conditions are applied to Eq. (40)

$$\begin{cases} t = 0 : p = p_e; \\ r \rightarrow \infty : p \rightarrow p_e; \\ z = z_0(r, t) : Q = -\frac{\langle k \rangle}{\mu_w} \frac{\partial \langle p \rangle}{\partial r} \end{cases} \quad (41)$$

The gas and two-phase regions are considered incompressible. The introduction of the dimensionless parameter Eq. (B3) and the self-similar variable Eq. (35) to Eq. (41) results to

$$\begin{cases} \xi = D_0 : \frac{d\langle P \rangle}{d\xi} = -\frac{1}{\Lambda(S=0)\xi}, \Lambda(S=0) = 1 \\ \xi \rightarrow \infty : \langle P \rangle \rightarrow P_e \end{cases} \quad (42)$$

The assumption of a low-compressible water phase yields the

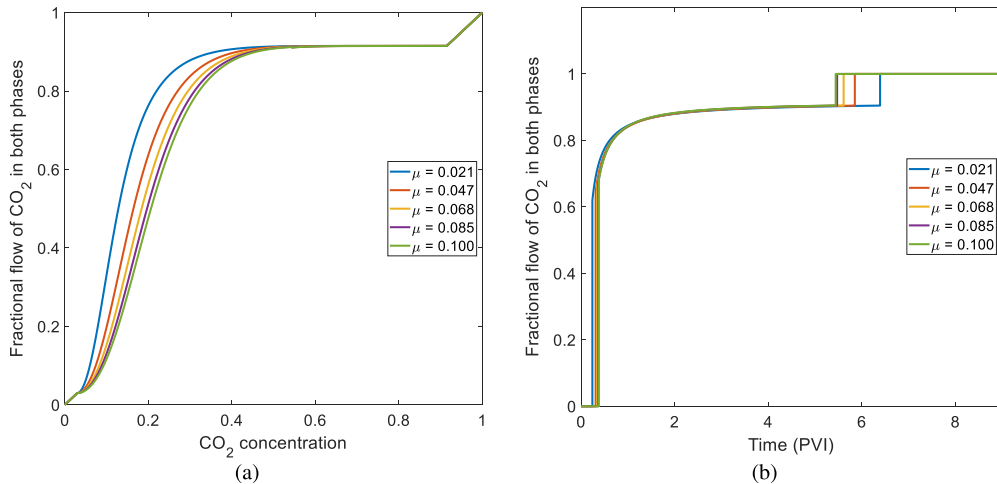


Fig. 5. (a) CO₂ fractional flow versus CO₂ concentration; (b) CO₂ fractional flow history at the outlet.

diffusivity equation Eq. (33). Details of the derivation is given in Appendix D. By imposing the boundary conditions Eq. (42) on Eq. (D10), the pressure distribution ahead of the water-gas front accounting for low water compressibility is

$$\langle P \rangle(\xi) = -e^{(AD_0)} Ei(-A\xi) + P_e \quad (43)$$

4.3. Calculations of total mobility in two-phase region

For large scale approximations, the dimensionless overall phase flux for water and gas is derived from Eq. (B4) as,

$$1 = -\Lambda(S)x \frac{\partial P}{\partial x} \quad (44)$$

where the total mobility is expressed as

$$\Lambda(S) = \left[\int_0^1 \frac{K(Z)k_{rg}(s)}{\mu[1 + \beta\Delta\sigma_{cr}(s)]} dZ - \int_0^1 K(Z)k_{rw}(s) dZ \right], \mu = \frac{\mu_g}{\mu_w} \quad (45)$$

The detailed derivations the expressions for total mobility in Zone 0, Zone 01 and Zone 1 are given by Eqs. (E5-E7) in Appendix E.

5. Explicit formulae for well injectivity and sweep efficiency

Based on the analytical model, presented in the previous section, the current section calculates pressure drawdown and well impedance (section 5.1) and sweep efficiency (section 5.2).

5.1. Calculations of pressure drop/well impedance

Based on Eq. (44), the pressure drop at any given moment (τ) is expressed as

$$\Delta P(\tau) = \int_{x_w}^{\infty} \left(-\frac{\partial P}{\partial x} \right) dx = \int_{x_w}^{\infty} \frac{1}{\Lambda(S)x} dx \quad (46)$$

At any given moment $\tau_i < \tau(D_0)$, three distinct regions exist: the gas zone, the two-phase zone, and the water zone ahead of the CO₂ front as shown in Fig. 3 and Fig. 7. The pressure drop for this moment is expressed as

$$\Delta P(\tau) = \int_{x_w}^{D_1\tau} \frac{1}{\Lambda(1)x} dx + \int_{D_1\tau}^{D_0\tau} \frac{1}{\Lambda(S)x} dx + \int_{D_0\tau}^{\infty} \frac{dP}{dx} dx = I_1 + I_2 + I_3 \quad (47)$$

where first, second and third integrals correspond to the single-phase gas zone, mixture zone, and single-phase water zone, respectively.

In single phase gas zone, the total mobility is equal to $\Lambda(1)$, hence, the pressure drop is expressed as

$$I_1 = \int_{x_w}^{D_1\tau} \frac{1}{\Lambda(1)x} dx \quad (48)$$

At the two-phase zone the pressure drop is expressed via the self-similar variable, ξ , where

$$d\xi = F'(C) dC \quad (49)$$

The introduction of the self-similar variable, Eq. (35) into the second integral of Eq. (47) yields the pressure drop in the two-phase zone as

$$I_2 = \int_{C_2}^{C_3} \frac{F'(C)}{F(C)\Lambda(C)} dC \quad (50)$$

For the low-compressible water zone ahead of the advanced front, the pressure drop is calculated from the solution (Eq. (43)) to the pressure diffusivity equation Eq. (D6) to obtain

$$I_3 = \int_{D_0\tau}^{\infty} -\frac{dP}{dx} dx = [P_e - e^{(AD_0)} Ei(-AD_0\tau)] - [P_e] = -e^{(AD_0)} Ei(-AD_0\tau) \quad (51)$$

Substituting Eqs. 48–51 into Eq. (47) gives the pressure drop at moment τ as

$$\Delta P(\tau) = \int_{x_w}^{D_1\tau} \frac{1}{\Lambda(1)x} dx + \int_{C_2}^{C_3} \frac{F'(C)}{F(C)\Lambda(C)} dC - e^{(AD_0)} Ei(-AD_0\tau) \quad (52)$$

Well impedance is the normalised reciprocal to injectivity index and can be expressed in terms of pressure drop as follows

$$J_w(\tau) = \frac{II(\tau=0)}{II(\tau)} = \frac{Q(\tau=0)}{\Delta P(\tau=0)} \frac{\Delta P(\tau)}{Q(\tau)} \quad (53)$$

The results of impedance and sweep calculations are presented in Fig. 6. Here we use the same fluid and rock properties as those presented at the end of section 4.1.

Blue curve in Fig. 6a shows the impedance decreases with time during the injection. Some increase in impedance due to fines migration is overly compensated by injection of gas with viscosity that is highly below the displaced water viscosity.

5.2. Sweep calculations

The ODE Eq. (30) allows for first integral. Let us integrate both sides of Eq. (30) over the domain Ω in the plane (x, τ) limited by characteristics with velocity D_0 and D_1 as shown in Fig. 7. Calculating double integral of both sides of Eq. (30) over the domain Ω using Green's theorem yields:

$$\iint \left[\frac{\partial C}{\partial \tau} + \frac{\partial F}{\partial x} \right] d\tau dx = \oint F d\tau - C dx = 0 \quad (54)$$

Accounting for the constancy of CO₂ concentration, C along the characteristics, the contour integral in Eq. (54) yields

$$\bar{C}(\tau) = (1 - x_w)C\left(\frac{1}{\tau}\right) - \tau F\left(C\left(\frac{1}{\tau}\right)\right) + \tau \quad (55)$$

where the average CO₂ concentration is given as

$$\bar{C}(\tau) = \int_{x_w}^1 C(x, \tau) dx \quad (56)$$

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

$$\bar{C}(\tau) = \tau \text{ with } C\left(\frac{1}{\tau}\right) = 0, F\left(C\left(\frac{1}{\tau}\right)\right) = 0 \quad (57)$$

At intermediate moments in time, $\left(\frac{1}{D_0} < \tau < \frac{1}{D_1}\right)$, the average CO₂ concentration is given as

$$\bar{C}(\tau) = (1 - x_w)C\left(\frac{1}{\tau}\right) - \tau F\left(C\left(\frac{1}{\tau}\right)\right) + \tau \quad (58)$$

At late moments, when stabilization is established $\left(\frac{1}{D_1} < \tau < \infty\right)$, the average CO₂ concentration is given as

$$\bar{C}(\tau) = (1 - x_w) \text{ with } C\left(\frac{1}{\tau}\right) = 1, F\left(C\left(\frac{1}{\tau}\right)\right) = 1 \quad (59)$$

Blue curve in Fig. 6b shows linear sweep growth before the breakthrough at the moment 0.2PVI, following slower increase during CO₂ production in two phases. Full evaporation occurs at the moment 6.4

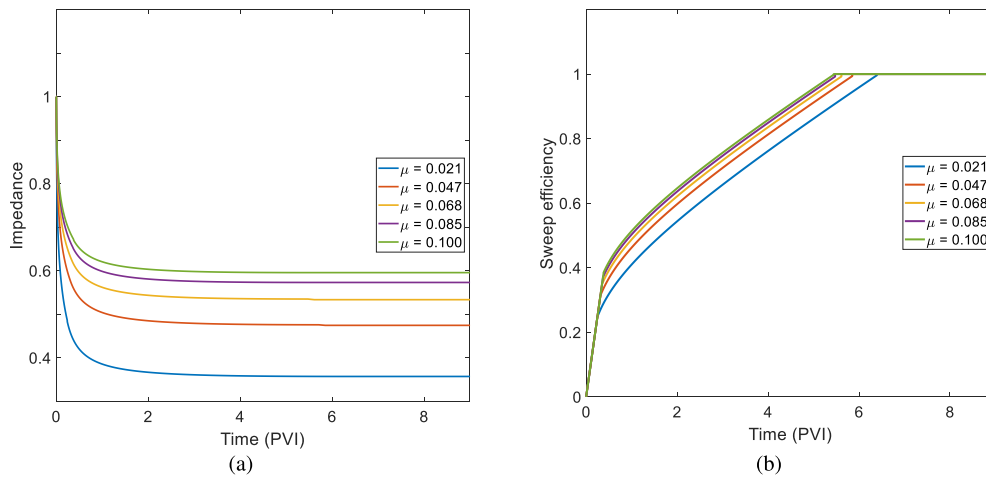


Fig. 6. (a) Impedance versus time; (b) Sweep efficiency versus time.

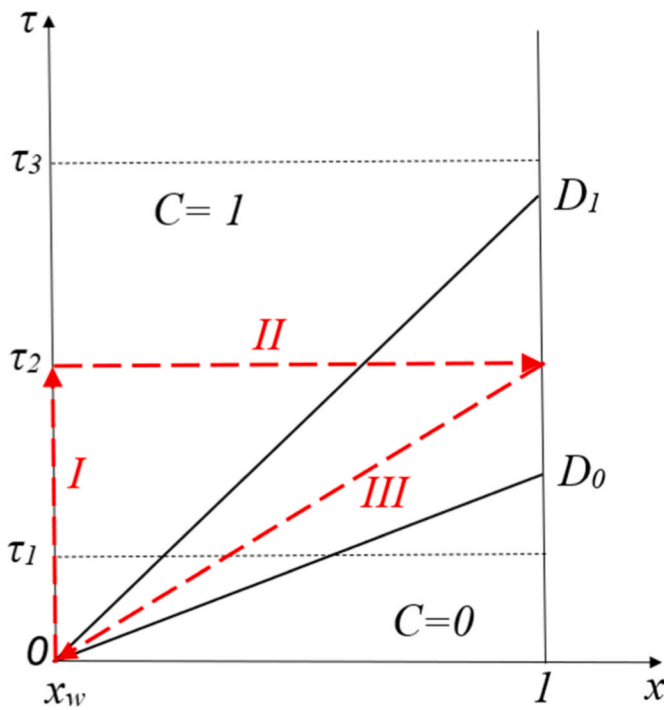


Fig. 7. Characteristic lines in the x - τ plane.

PVI.

5.3. Step-by-step procedure for practical engineering calculations

This section presents the detailed step-by-step procedure/algorithm for numerical implementation of the analytical model. The model facilitates the prediction of CO₂ behaviour by assessing essential metrics such as CO₂ distribution in the layer-cake system, sweep efficiency, impedance and the ability to implement multivariate sensitivity analysis. The steps comprise the following.

i. Input data

- Define the depth-dependent permeability profile $k(z)$: specify an analytical formula (for example, third order polynomial in Eq. (38), or piecewise constant, etc) and set all coefficient values.

- Define coefficients of Brooks power-law formula for Leverett function (capillary pressure expression by Eq. 5).
 - Define coefficients of Corey relative permeability functions in Eq. (39).
 - Determine equilibrium concentrations for binary water-CO₂ mixture c_g and c_w at constant reservoir pressure and temperature.
 - Determine densities and viscosities of water and CO₂ at constant reservoir pressure and temperature.
 - Set the coefficients σ_0 and B for maximum retention function (Eq. (6)) and formation damage coefficient β (Eq. (8)).
- #### ii. Calculations of average fractional flow for CO₂ $F=F(C)$
- Determine whether the reservoir is thin or thick using Eq. (14).
 - Discretise the parameter space: divide the intervals $[0,1]$ for average gas saturation S and the ranges of front positions z_0 and z_1 , each into N equal sub-intervals.
 - For zones 0 and 01 (parameterized by z_0): compute averaged overall CO₂ concentration $C(z_0)$ as a function of z_0 at each $N-1$ interior point using the formula from second row and third column in Table 1 or Table 2 for thick or thin reservoirs, respectively.
 - Calculate fractional flow for gas phase f as a function of z_0 in $N-1$ points using formula from second row and fourth column in Table 1 or Table 2 for thick or thin reservoirs, respectively, for zones 0 and 01.
 - Calculate overall fractional flow of CO₂ $F(C)$ as a function of z_0 in $N-1$ points using Eq. (26), for zones 0 and 01.
 - For zone 1 (parameterized by z_1): compute averaged overall CO₂ concentration $C(z_1)$ as a function of z_1 at each $N-1$ interior point using formula from fourth row and third column in Table 1 or Table 2 for thick or thin reservoirs, respectively.
 - Calculate fractional flow for gas phase f as a function of z_1 in $N-1$ points using formula from fourth row and fourth column in Table 1 or Table 2 for thick or thin reservoirs, respectively, for zone 1.
 - Calculate overall fractional flow for CO₂ $F(C)$ as a function of z_1 in $N-1$ points using Eq. (26), for region 1.
- #### iii. Calculations of average CO₂ concentration, fractional flow for CO₂, and sweep efficiency
- Calculate derivative array $dF/dC = (F_{n+1}-F_n)/(C_{n+1}-C_n)$ for all $n = 0,1,2 \dots N-1$. These are characteristic velocities of the self-similar solution Eq. (36).
 - Determine advanced and receded front velocities D_0 and D_1 from Eq. (37).
 - Calculate average CO₂ concentration profiles $C(x/\tau_k)$ for moments $\tau_1, \tau_2 \dots$ using Eq. (36).

- Calculate fractional flow of CO₂ at $x = 1$ for moments $\tau_1, \tau_2 \dots$ using corresponding values of C .
 - Calculate moments $\tau_n = (C_{n+1} - C_n) / (F_{n+1} - F_n)$ for all values $n = 0, 1, 2 \dots N-1$.
 - Calculate values of sweep efficiency $\bar{C}(\tau_n)$ using Eqs. 57, 58, and 59.
- iv. Calculations of pressure drawdown and well impedance
- Compute the total two-phase mobility using Eq. (E4) in Appendix E
 - Before the arrival of the advanced front for $\tau < 1/D_0$, calculate I_3 using Eq. (51), I_2 – Eq. (50), and I_1 – Eq. (48) and calculate pressure drawdown as the sum of I_1 , I_2 and I_3 (Eq. (52)) for moments τ_l , $l = 1, 2 \dots$
 - After the arrival of the advanced front for $1/D_1 < \tau < 1/D_0$, calculate I_1 and I_2 only and calculate the pressure drawdown as the sum of I_1 and I_2 for moments τ_l , $l = 1, 2 \dots$
 - Calculate well impedance using Eq. (53).

6. Downscaling

The downscaling procedure determines the vertical distribution of gas saturation s and CO₂ c from the overall CO₂ concentration $C(x, \tau)$ obtained through the analytical solution Eq. (36). The vertical saturation profile $s(z)$ is given by Eq. (19), which expresses s as a function of depth z through the inverse of the capillary pressure equation Eq. (18). The corresponding microscale CO₂ concentration $c(z)$ follows from substituting $s(z)$ into Eq. (2), yielding the depth distributions described by Eqs. (20) and (22) parameterized by z_0 and z_1 , respectively. The downscaling is performed by using the analytical model for upscaled flow Eq. (36) to determine depth CO₂ concentration or phase saturation distributions by using the inverse expression

$$Z_0(x, \tau) = \chi_0(C), Z_1(x, \tau) = \chi_1(C) \quad (60)$$

where χ_0 and χ_1 are the inverse equations of the averaged equations 20 and 22, respectively.

Fig. 8a shows the case of permeability increasing with depth, Fig. 8b – depth decreasing permeability. Viscous forces direct the injected gas into highly permeable layers. Buoyancy forces gas upwards. In the case of permeability increasing with depth, both viscous and gravitational forces move gas upwards. So, gas saturation decrease with depth is expected. Indeed, in Fig. 9a, where saturation variation with depth is presented for 7 moments, gas saturation decreases with depth.

In cases where permeability decreases with depth, viscous forces tend to direct the injected gas into the lower reservoir layers, while gravitational forces drive the gas upward. The interplay between these opposing forces results in non-monotonic vertical saturation profiles. As illustrated in Fig. 9b gas saturation increases from the reservoir bottom upward, reaching a maximum at an intermediate depth, and subsequently decreases toward the reservoir top. At each depth, saturation monotonically increases with time.

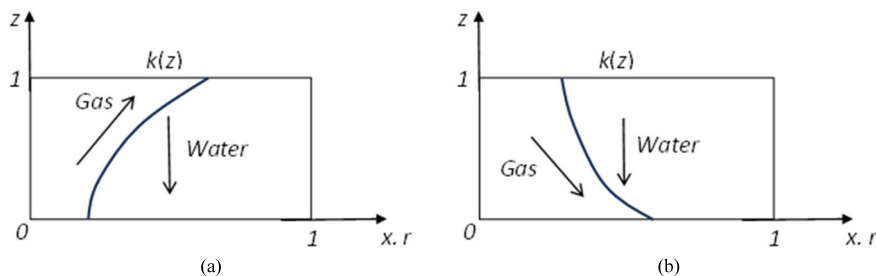


Fig. 8. Illustration of flow regimes for layer cake system with (a) Permeability decreasing with depth; (b) Permeability increasing with depth.

7. Sensitivity analysis

This section presents sensitivity study of water displacement by injected CO₂ versus reservoir heterogeneity, viscosity ratio, concentration of detachable fines, formation damage coefficient and power law exponent for straining.

Heterogeneity – Here we use the relative range, ν , that is equal to the difference between maximum and minimum permeability divided by its mean value. The relative range expresses the spread of permeability values relative to the average; a higher relative range indicates higher heterogeneity, while a lower relative range implies more uniform permeability. Fig. 10a shows that the more heterogeneous is the reservoir, the higher is the fractional flow and the more concave is the fractional flow curve. Consequently, the higher is the gas cut (Fig. 10b). Fig. 10b-d show that increase in heterogeneity decrease breakthrough period from 0.4PVI to 0.2PVI, increase the evaporation period from 3.5PVI to 4.5PVI, decrease sweep by 35% and decrease the stabilized impedance from 0.45 to 0.36.

The curvilinearity increase (Fig. 10a) results to the decrease of tangent D_1 and increase in tangent D_0 . So, increase in heterogeneity decreases breakthrough time, $1/D_0$ and increases the evaporation period, $1/D_1$, as shown in Fig. 10b and c. However, even for very concave FFC, D_1 value is lower than the tangent of the straight-line segment 1-L in Fig. 4b; D_0 cannot exceed the tangent of the straight-line segment 0-L

$$D_0 > \frac{1 - c_w}{c_g}, D_1 < \frac{c_w}{1 - c_g} \quad (61)$$

Consequently, breakthrough time is lower than $c_g/(1 - c_w)$, and the evaporation period is above $(1 - c_g)/c_w$. The higher is the heterogeneity, the lower is the sweep (Fig. 10c) and the lower is the impedance (Fig. 10d).

Viscosity ratio – Fig. 5a presents the plots of fractional flow functions $F(C)$ for various viscosity ratios $\mu = \mu_g/\mu_w$. Here the viscosity ratio increases from 0.021 typical for gaseous CO₂ up to 0.1 for supercritical CO₂. The higher is the gas viscosity, the lower is its fractional flow. The single-phase regions for fractional flow functions are independent of phase viscosities. Fig. 5b shows the corresponding breakthrough gas-cuts ($F(C)$) versus PVI at $x = 1$. The higher is the gas viscosity, the higher is its fraction at the outlet. Consequently, the higher is the viscosity ratio, the higher is the sweep efficiency (Fig. 6b). With the overall viscosity ratio increase, the sweep efficiency of the heterogeneous reservoir increases by 0.1, which is quite significant. Simultaneously, the stabilized well impedance increases approximately twice (Fig. 6a).

Concentration of detachable fines – Fig. 11 shows the effects of total concentration of detachable fines. The higher is the detachable fines concentration, the higher is the concentration of strained fines and the consequent formation damage to gas phase and gas deceleration. Fig. 11a shows that increase in σ_0 yields increase in breakthrough time and decrease in evaporation period. It also yields the increase in sweep by 0.14 with the overall σ_0 increase from 5×10^{-5} to 4×10^{-3} , (Fig. 11b). Overall increase in detachable fines concentration results in impedance increase; the stabilized values increase 1.75 times.

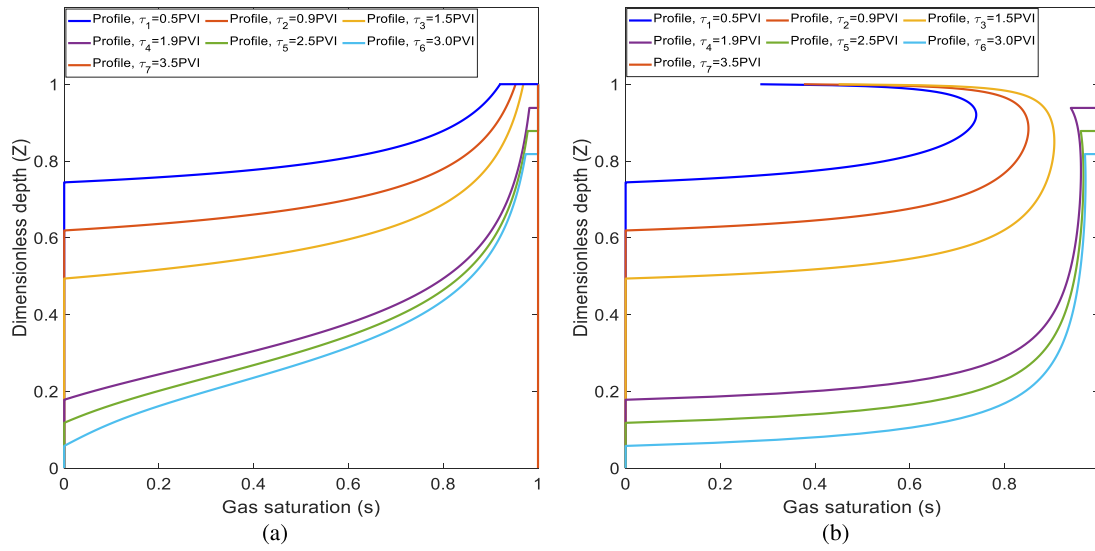


Fig. 9. Downscale saturation distribution versus vertical coordinate at different moments; (a) permeability decreasing with depth, (b) permeability increasing with depth.

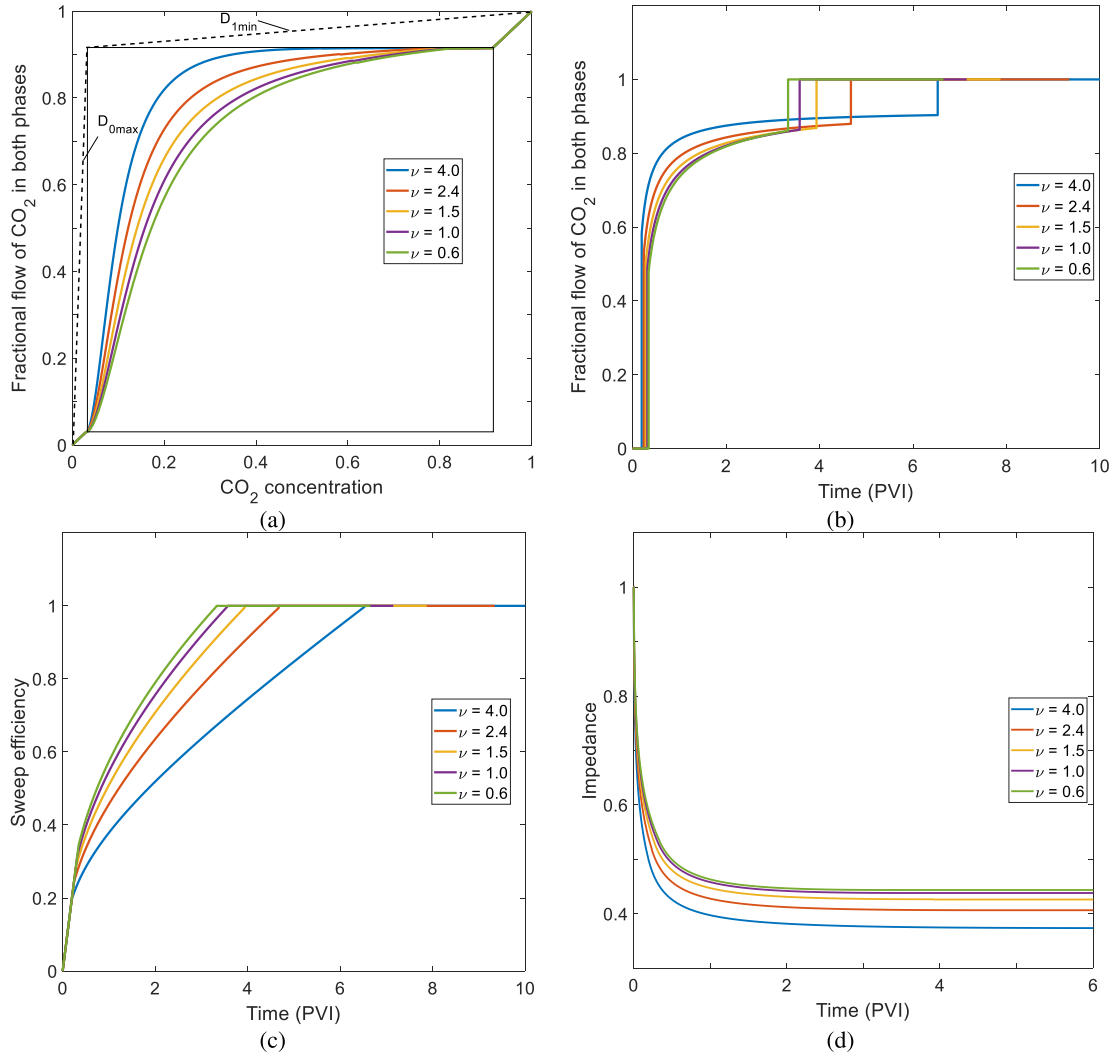


Fig. 10. Effect of the reservoir heterogeneity on CO₂ injection into aquifers: (a) CO₂ fractional flow versus CO₂ concentration; (b) CO₂ fractional flow history at the outlet; (c) Sweep efficiency versus time; (d) Impedance versus time.

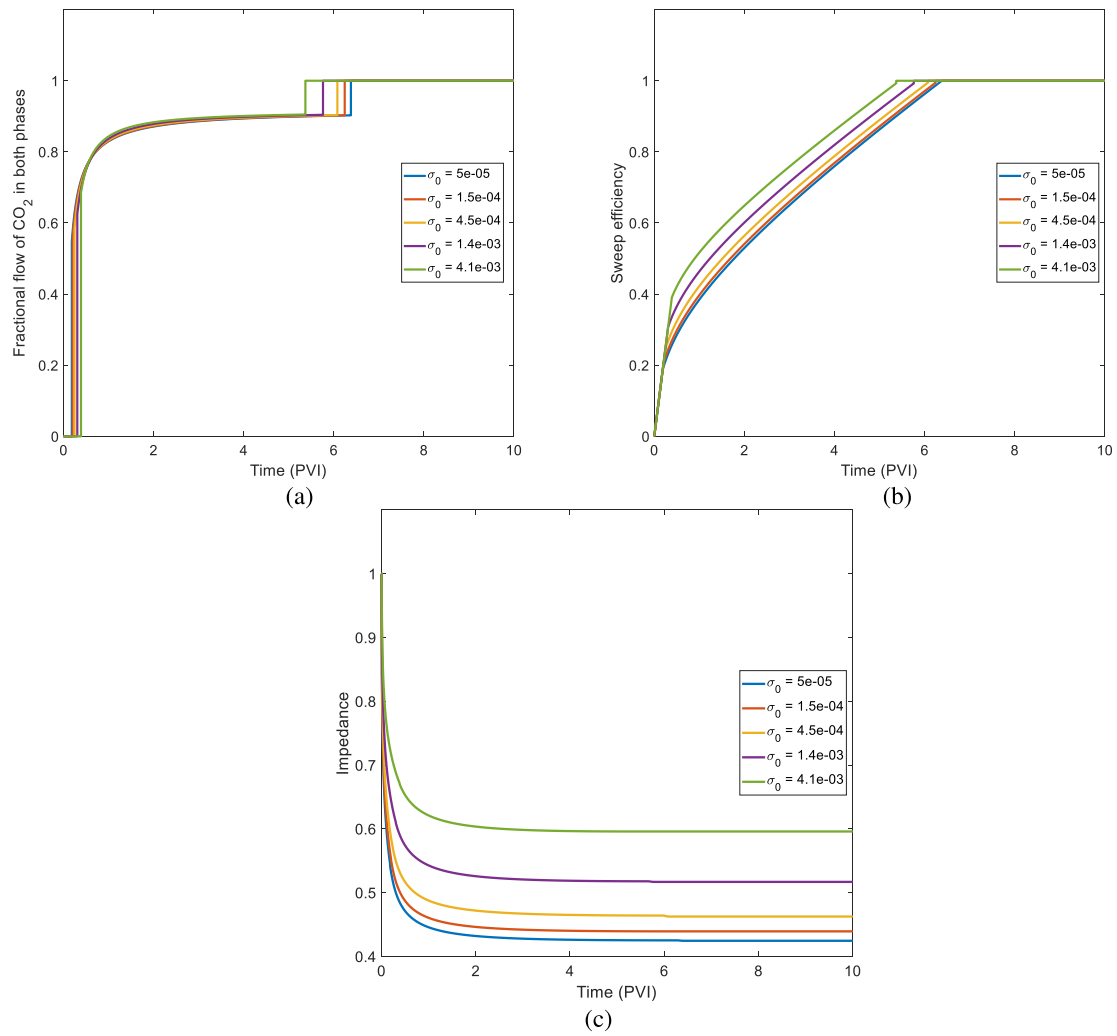


Fig. 11. (a) CO₂ fractional flow history at the outlet; (b) Sweep efficiency versus time; (c) Impedance versus time with varying concentration of detachable fines.

Formation damage coefficient – The concentration of detachable fines σ_0 and formation damage coefficient β are expressed as product in Eq. (6). As a result, increasing σ_0 has the same effect as increasing β ; for example, a hundredfold increase in σ_0 is equivalent to a hundredfold increase in β . Fig. 12a demonstrates that increasing the formation damage coefficient from zero to 30,000 extends the breakthrough period from 0.2 PVI to 0.4 PVI, and reduces the evaporation period from 6.8 PVI to 5.8 PVI. Additionally, as shown in Fig. 12b, this increase in β leads to 30% improvement in sweep efficiency and raises the stabilized impedance from 0.34 to 0.58.

Power law exponent for strained fines – Eq. (6) shows that the higher is the power law exponent B , the higher is the MRF, and the higher is the damage to gas phase. Fig. 13 shows that increase of power law B yields increase in sweep efficiency by 11% (Fig. 13b), increase in breakthrough period and decrease in overall evaporation period (Fig. 13a) and increase in stabilized impedance from 0.45 to 0.52 (Fig. 13c).

8. Discussions

In this section we discuss the restrictions of the developed analytical model for predicting of CO₂ storage in saline aquifers, its validity and applicability.

Analytical model validity The conditions under which the classical VE model is valid have been well established both theoretically and through validation against two-dimensional (2D) and three-dimensional (3D)

reservoir simulations. The numerous references are available from books (Bedrikovetsky, 2013; Lake et al., 2014; Bruining, 2021) and the referred papers by (Alamara et al., 2023a, 2023b, 2023c, 2025a, 2025b). Compared with the classical VE model, the present model (34) introduces permeability damage due to fines migration by dividing the expression for undamaged gas permeability by formation damage factor $1 + \beta \Delta \sigma_{crs}$, Eq. (8). The validity of this procedure to model fines migration has been rigorously validated by comparison with three sets of lab tests (Nguyen et al., 2022) and by matching field data (Russell et al. 2025). Another extension of the classical VE model, provided by the present model (34), is partial miscibility of water and CO₂ expressed by two thermodynamic constants c_w and c_g . However, after the averaging, a new model, like the classical VE model, is expressed in fractional flow form, Eq. (34). Thus, the extension of the VE model to account for partial CO₂-water miscibility and fines migration does not introduce additional restrictions beyond those imposed by the traditional VE framework.

Applicability of the analytical model The analytical model (36, 37) in large scale approximation is applicable for practical predictions of geological CO₂ storage behavior subject to the following assumptions: layer-cake heterogeneity with radial homogeneity; Amagat's law for binary mixture with incompressible water and CO₂ components; pressure drawdown and Joule-Thomson temperature variation are significantly lower than the average reservoir pressure and temperature; constant equilibrium concentrations of water in gas c_w and CO₂ in water c_g ; vertical and lateral variation of gas density are significantly smaller

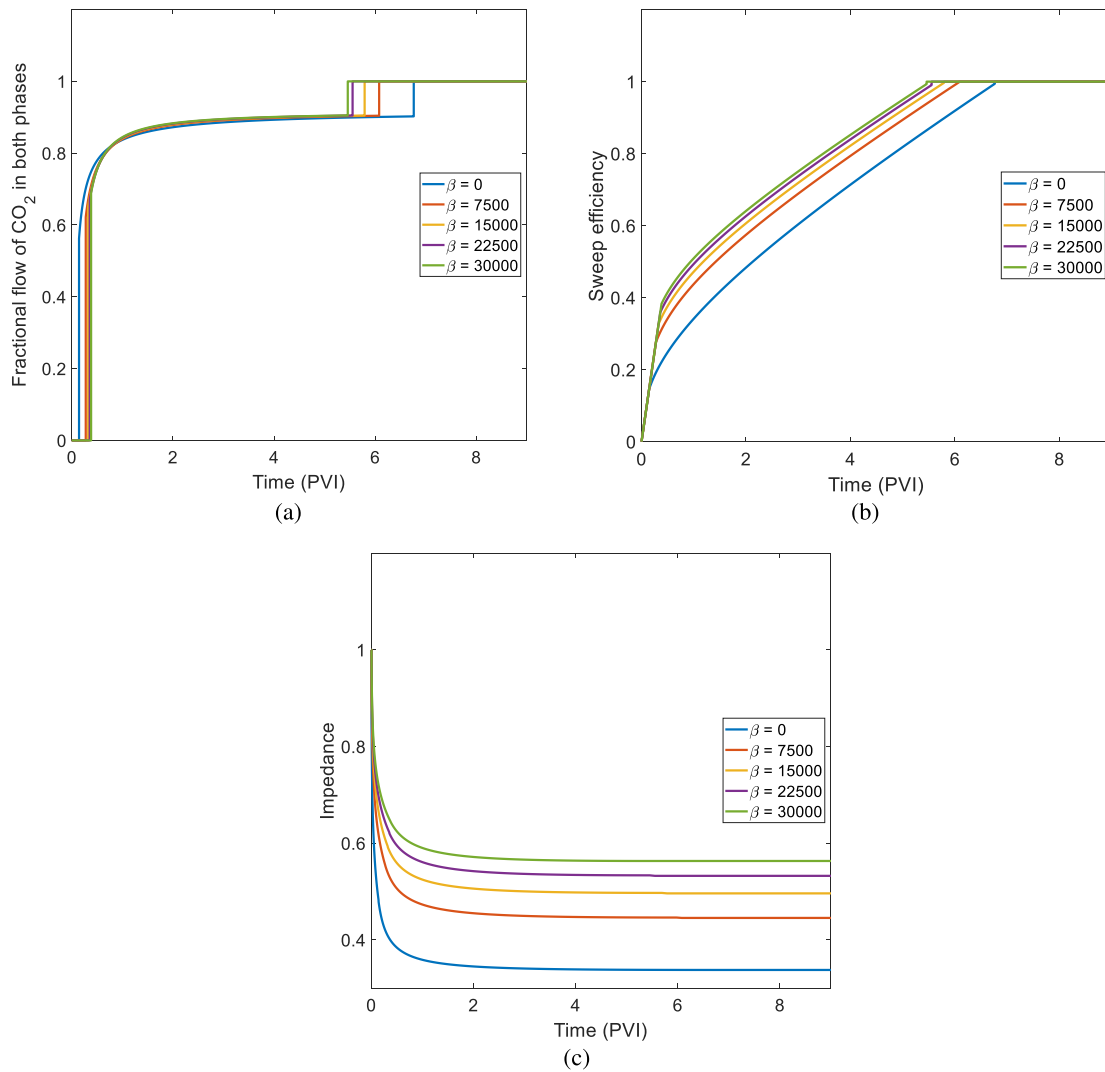


Fig. 12. (a) CO₂ fractional flow history at the outlet; (b) Sweep efficiency versus time; (c) Impedance versus time with varying damage coefficient.

than the average gas density; constant viscosities of water and gas; detachment of reservoir fines by capillary force exerting the attached particles from the gas-water menisci and instant capture of mobilized fines by the rock.

The model assumes a radially homogeneous reservoir with constant thickness H . Assuming low variation of $H(r)$ yields horizontal fluxes in all layers. Hydrostatic pressure distributions, given by Eq. (3) leads to z -independent gradients of both fluxes. The averaging defined in Eq. (B1) permits both pressure gradients to be taken outside the integral, enabling the introduction of pseudo-phase permeabilities that are r -dependent. Consequently, the fractional flow, calculated as in Eq. (25), depends on both saturation S and radial position r . The final equation of conservation law (30) with r -dependent fractional flow allows for exact solution (Prempeh et al., 2024; Shokrollahi et al., 2025). This solution is not self-similar anymore, yielding more complex calculations of sweep efficiency and well impedance.

Laboratory core flooding experiments, involving CO₂ injection into brine-saturated cores, typically exhibit between 0.5×10^4 and 2.0×10^4 PVIs during the full evaporation period (Keykhosravi et al., 2025). In contrast, the large-scale VE model presented in Eq. (31) describes the full evaporation period as $1/D_1$, where the period typically varies within the range of $[10, 10^3]$. The discrepancy between these scales arises from the differing nature of the two processes: core flooding experiments are conducted under non-equilibrium evaporation conditions, while

large-scale reservoir displacement follows the assumptions of the large-scale approximation, as outlined by previous work (Bedrikovetsky, 2013). The large-scale VE model, Eq. (31) does not account for capillary pressure effects, which could influence fluid distribution within the reservoir. With capillary pressure, Eq. (25) allows for exact self-similar solution, where initial saturation is achieved asymptotically as the radius approaches infinity. Obtaining this solution is the topic of forthcoming research.

Several studies by F. Hussain and collaborators have investigated the effects of CO₂ humidity on reservoir sweep efficiency and plume propagation, particularly in the context of CO₂ injection with equilibrium vapor concentrations (Ajoma et al., 2021; Yin et al., 2023, 2025a, 2025b). To assess the impact of CO₂ humidity on the displacement behaviour in layer-cake reservoirs, the current VE model (Eq. (31)) would need to be extended to account for injected CO₂ with vapor content. This extension is crucial for improving the model's predictive capability in reservoirs where CO₂ injection with significant vapor content may alter the displacement dynamics.

The analytical model is presented by explicit formulae in Table 1, Table 2 and Eqs. 36 and 37. This allows for direct implementation of the model in MATLAB or Excel without going through the mathematical derivations.

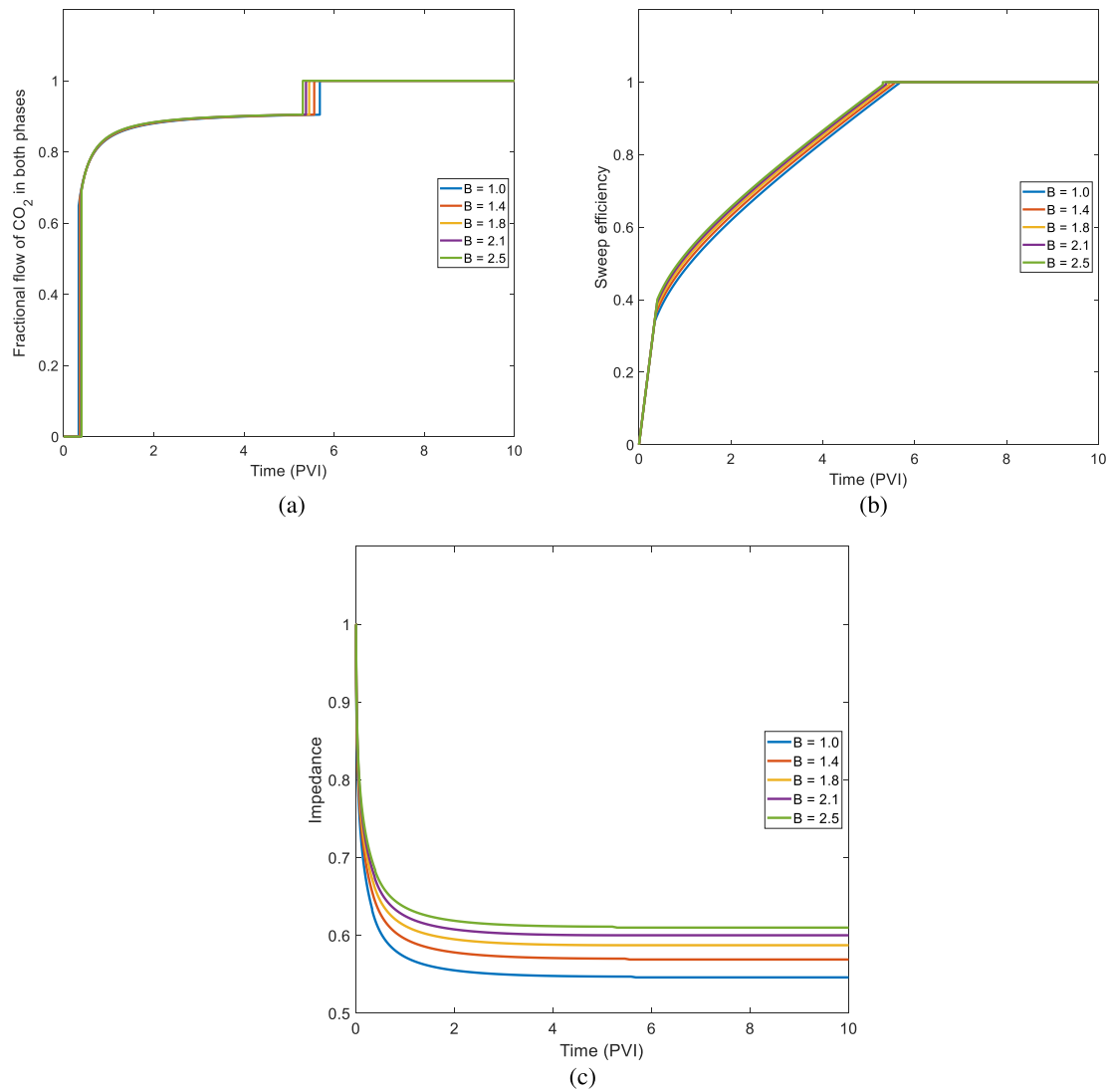


Fig. 13. (a) CO_2 fractional flow history at the outlet; (b) Sweep efficiency versus time; (c) Impedance versus time with varying power law exponent for straining.

9. Conclusions

Analytical modelling of radial, pseudo-2D displacement of brine by CO_2 , accounting for reservoir heterogeneity, partial water-gas miscibility, and fines migration, leads to the following key conclusions.

The vertical capillary-gravity equilibrium (VE) model for two-phase flow in layer-cake reservoirs can be extended to incorporate water evaporation into the injected gas, CO_2 dissolution in formation brine, and fines migration with associated permeability damage. The extended VE formulation for unknown averaged CO_2 concentration $C(r, t)$ is mathematically equivalent to a 1D model of partially miscible displacement of binary mixtures with mobile fines in a homogeneous formation. The VE model for unknown pressure $p(r, t)$ for incompressible flow can be matched to the initial reservoir pressure by introducing slight compressibility in the reservoir fluid ahead of the displacement front, enabling continuity of pressure across regions.

The quasi-2D vertically averaged model allows for an exact self-similar solution, yielding explicit formulae for phase saturations, CO_2 concentration, and pressure. This analytical solution also provides explicit formulae for estimating sweep efficiency (storage capacity) and well injectivity, enabling rapid multivariant sensitivity study and parametric evaluations.

Downscaling of the 1D solution reconstructs vertical (z -dependent) profiles of saturation and concentration as functions of radial position

and time. This is achieved through parameterization of depth-dependent distributions based on the averaged flow variables. Downscaling of vertical CO_2 -concentration and saturation distribution in the reservoirs with the permeability decreasing with depth yields monotonic CO_2 -concentration and saturation distributions. If the permeability increases with depth, CO_2 -concentration and saturation distribution can be non-monotonic, which is attributed to the force competition between gravity and pressure gradient.

Sensitivity analysis reveals that CO_2 -brine viscosity ratio, permeability heterogeneity, and fines migration significantly influence storage performance and injectivity. Increased permeability damage reduces injectivity but enhances storage capacity due to improved sweep.

Higher permeability heterogeneity leads to earlier gas breakthrough and a longer evaporation period. However, for any depth-dependent permeability distribution $k(z)$, breakthrough time remains below $c_g/(1-c_w)$, while the duration of the evaporation period exceeds $(1-c_g)/c_w$.

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CRediT authorship contribution statement

Kofi Ohemeng Kyei Prempeh: Investigation, Methodology, Software, Validation, Visualization, Writing – original draft, Writing – review & editing. **Rouhi Farajzadeh:** Methodology, Supervision, Validation, Writing – original draft. **Pavel Bedrikovetsky:** Methodology, Supervision, Writing – original draft.

Declaration of competing interest

The authors declare that they have no known competing financial

interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Depth density variation of CO₂

Let us estimate the CO₂ density difference between the top and bottom of the reservoir. We consider a reservoir of thickness $H = 25$ m at a depth of 3 km, where pressure is 30 MPa and temperature 100°C (373K). Using critical properties of CO₂ - critical temperature $T_{cr} = 300$ K, critical pressure $p_{cr} = 7.4$ MPa, and acentric factor $\omega = 0.22$ – and applying the Peng-Robinson equation of state (EoS), we obtain the temperature-dependent attractive parameter $a(T) = 0.29$ and CO₂ density of $\rho_g = 800$ kgm⁻³. The hydrostatic pressure drop across the reservoir thickness H is

$$\Delta p = \rho_g g H = 800 \times 9.81 \times 25 \approx 2 \times 10^5 \text{ Pa} \quad (\text{A1})$$

The isothermal compressibility is calculated as

$$k_T = -\frac{1}{V} \left(\frac{\partial p}{\partial V} \right)_T^{-1} \approx 10^{-9} \text{ Pa}^{-1} \quad (\text{A2})$$

which is approximately equal to the data provided by Lemmon et al. (2018).

The ratio between CO₂ density difference between the reservoir top and bottom and average CO₂ density for $k_T = 10^{-9} \text{ Pa}^{-1}$ is

$$\frac{\Delta \rho_g}{\rho_g} = k_T \Delta p = 10^{-9} \times 2 \times 10^5 = 2 \times 10^{-4} \quad (\text{A3})$$

So, the supercritical CO₂ density, under the above-mentioned conditions, can be assumed constant over the vertical. For the case where pressure drawdown is significantly lower than the average reservoir pressure, the lateral pressure and gas density variations are negligible. Therefore, in the present work, as in the classical VE model, gas density is assumed to be constant. This explains frequent application of the classical VE model for reservoir simulation of CO₂ storage in aquifers (Nordbotten and Celia, 2006, 2011; Alamara et al., 2023a, 2023b, 2023c, 2025a, 2025b; Gasda et al., 2009).

Appendix B. Overall gas and water fluxes

Under the assumption of hydrostatic pressure distribution in both phases, Eq. (3), pressure gradients are independent of the vertical coordinate z . The overall phase fluxes of water and gas in the radial direction are obtained by integration of Eq. (8) over reservoir thickness

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

Taking the sum of the phase velocities in Eq. (B1) and expressing the result in terms of pressure in water and the capillary pressure yields

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

Let us introduce dimensionless variables and parameters:

$$x = \frac{r^2}{r_e^2}, Z = \frac{z}{H}, \tau = \frac{Q t}{\phi \pi r_e^2}, h_c = \frac{H_c}{H}, \varepsilon_c = \frac{4\pi k_0 H}{Q \mu_w} \frac{\sigma \cos \theta \sqrt{\phi}}{\sqrt{k_0}}, \kappa = \frac{4\pi k_0}{Q c_t \mu_w}, \langle p \rangle = \frac{1}{H} \int_0^H p(r, z, t) dz \quad (\text{B3})$$

$$P = \frac{4\pi k_0 H}{Q \mu_w} p, P_w = \frac{4\pi k_0 H}{Q \mu_w} p_w, k_0 = \frac{1}{H} \int_0^H k(z) dz = \int_0^1 k(Z) dZ, k(Z) = k_0 K(Z), \int_0^1 K(Z) dZ = 1$$

Based on the dimensionless variables and parameters in Eq. (B3), the dimensionless form of the overall phase flux for water and gas is obtained as:

$$1 = - \left[\int_0^1 K(Z)k_{rw}(s) dZ + \int_0^1 \frac{K(Z)k_{rg}(s) dZ}{\mu[1 + \beta \Delta \sigma_{cr}(s)]} \right] x \frac{\partial P_w}{\partial x} - \varepsilon_c \int_0^1 \frac{K(Z)k_{rg}(s) dZ}{\mu[1 + \beta \Delta \sigma_{cr}(s)]} x \frac{\partial J(s)}{\partial x} \quad (\text{B4})$$

Substituting Eq. (B1) into the second equation of Eq. (2) yields the overall flux of CO₂-component in dimensional and dimensionless forms

$$U_g = -(1 - c_w) \int_0^H \frac{k(z)k_{rg}(s)dz}{\mu_g[1 + \beta\Delta\sigma_{cr}(s)]} \frac{\partial p_g}{\partial r} - c_g \int_0^H \frac{k(z)k_{rw}(s)dz}{\mu_w} \frac{\partial p_w}{\partial r} \quad (B5)$$

$$\frac{U_g}{U} = -(1 - c_w) \int_0^1 \frac{K(Z)k_{rg}(s)dZ}{\mu[1 + \beta\Delta\sigma_{cr}(s)]} x \frac{\partial P_g}{\partial x} - c_g \epsilon_c \int_0^1 K(Z)k_{rw}(s)dZ x \frac{\partial J(s)}{\partial x}$$

Expressing Eq. (B5) in terms of water and capillary pressure gradients gives

$$\frac{U_g}{U} = - \left[(1 - c_w) \int_0^1 \frac{K(Z)k_{rg}(s)dZ}{\mu[1 + \beta\Delta\sigma_{cr}(s)]} + c_g \int_0^1 K(Z)k_{rw}(s)dZ \right] x \frac{\partial P_w}{\partial x} - (1 - c_w) \epsilon_c \int_0^1 \frac{K(Z)k_{rg}(s)dZ}{\mu[1 + \beta\Delta\sigma_{cr}(s)]} x \frac{\partial J}{\partial x} \quad (B6)$$

Determining the expression for water pressure gradient from Eq. (B2) and substituting the results into Eq. (B5) gives the overall flux of CO₂ component in dimensional and dimensionless forms

$$U_g = \frac{(1 - c_w)\lambda_g(S) + c_g\lambda_w(S)}{\lambda(S)} U + \left\{ \frac{(1 - c_w)\lambda_g(S) + c_g\lambda_w(S)}{\lambda(S)} \lambda_g(S) - (1 - c_w)\lambda_g(S) \right\} \frac{\partial p_c}{\partial r} \quad (B7)$$

$$\frac{U_g}{U} = \frac{[(1 - c_w)\Lambda_g(S) + c_g\Lambda_w(S)]}{\Lambda(S)} + \left\{ \frac{[(1 - c_w)\Lambda_g(S) + c_g\Lambda_w(S)]\Lambda_g(S)}{\Lambda(S)} - (1 - c_w)\Lambda_g(S) \right\} x \epsilon_c \frac{\partial J}{\partial x}$$

where the mobility of gas, water and total mobility are expressed in dimensional and dimensionless forms

$$\lambda_g(S) = \int_0^H \frac{k(z)k_{rg}(s)dz}{\mu_g[1 + \beta\Delta\sigma_{cr}(s)]}, \lambda_w(S) = \int_0^H \frac{k(z)k_{rw}(s)dz}{\mu_w}, \lambda(S) = \lambda_g(S) + \lambda_w(S) \quad (B8)$$

$$\Lambda_g(S) = \int_0^1 \frac{K(Z)k_{rg}(s)dZ}{\mu[1 + \beta\Delta\sigma_{cr}(s)]}, \Lambda_w(S) = \int_0^1 K(Z)k_{rw}(s)dZ, \Lambda(S) = \Lambda_g(S) + \Lambda_w(S)$$

Eq. (B6) are used in section 3.2 to derive averaged mass balance equation (28) for displacement water by CO₂.

Appendix C. 1D Averaged mass balance for gas

The 1D mass balance for displacement of water by gas through a layer cake system under vertical equilibrium is expressed as

$$\phi \frac{\partial C}{\partial t} + \frac{1}{r} \frac{\partial(rU_g)}{\partial r} = 0 \quad (C1)$$

Substituting the expression for overall CO₂ gas flux Eq. (27) into the mass balance Eq. (C1) gives

$$\phi \frac{\partial C}{\partial t} + \frac{1}{r} \frac{\partial}{\partial r}(rUF) = - \frac{1}{r} \frac{\partial}{\partial r} \left[r(F - (1 - c_w)) \int_0^H \frac{k(z)k_{rg}(s)dz}{\mu_g(1 + \beta\Delta\sigma_{cr}(s))} \frac{\partial p_c(s)}{\partial r} \right] \quad (C2)$$

Introducing the dimensionless variables and parameters (B3) into Eq. (C2) results in the dimensionless equation for two phase flow of partly miscible fluids, Eq. (28) presented in the main text.

Appendix D. Pressure distribution ahead of the water-gas front accounting for water compressibility

Let us show that 2D single-phase low-compressible flow under vertical gravity equilibrium can be averaged in z , yielding traditional 1D pressure-diffusivity equation. The 2D mass balance equation for low-compressible water ahead of the advanced front is

$$\frac{\partial}{\partial t}(\phi\rho_w) + \frac{1}{r} \frac{\partial}{\partial r}(r\rho_w v_{wr}) + \frac{\partial}{\partial z}(\rho_w v_{wz}) = 0 \quad (D1)$$

Under the assumption of vertical equilibrium (second Eq. (3)), the velocity of water in the vertical direction v_{wz} is equal zero. Hence the mass balance equation for low-compressible water, Eq. (D1) reduces to

$$\frac{\partial}{\partial t}(\phi\rho_w) + \frac{1}{r} \frac{\partial}{\partial r}(r\rho_w v_{wr}) = 0 \quad (D2)$$

Substitution of the Darcy law for water Eq. (8) and expression for total compressibility Eq. (9) into Eq. (D2) and neglecting pressure dependency of water density in the mass transfer term yields

$$c_t \phi_0 \frac{\partial p}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{k(z)}{\mu_w} \frac{\partial p}{\partial r} \right) \quad (D3)$$

In this form, z acts as a parameter. Let us introduce averaged pressure in the brine-flow zone

$$\langle p \rangle(r, t) = \frac{1}{H} \int_0^H p(r, z, t) dz \quad (D4)$$

Assuming pressure independence of water density in hydrostatic expression (3) yields z -independence of time- and radius-derivatives of pressure. Therefore, time- and radius-derivatives of pressure are equal to those of average pressure. Integrating Eq. (D4) across z yields

$$\frac{\partial \langle p \rangle}{\partial t} = \frac{1}{H c_t \phi_0 \mu_w} \frac{1}{r} \frac{\partial}{\partial r} \left[r \left(\int_0^H k_h(z) dz \right) \frac{\partial \langle p \rangle}{\partial r} \right] \quad (D5)$$

Finally, single-phase low-compressible flow under hydrostatic pressure distribution is described by pressure-diffusivity equation with average permeability.

Solution of outflow problem Introducing the dimensionless variables and parameters Eq. (B3) into Eq. (D5) yields the dimensionless form of the pressure diffusivity as

$$\frac{\partial}{\partial x} \left(x \frac{\partial \langle P \rangle}{\partial x} \right) = A \frac{\partial \langle P \rangle}{\partial \tau}, \quad A = 1/\kappa \quad (D6)$$

The introduction of the self-similar variable in Eq. (35) into Eq. (D6) yields a second order ordinary differential equation given as

$$\frac{d \langle P \rangle}{d \xi} + \xi \frac{d^2 \langle P \rangle}{d \xi^2} = -A \xi \frac{d \langle P \rangle}{d \xi} \quad (D7)$$

The order of Eq. (D7) is reduced by introducing $v = \frac{d \langle P \rangle}{d \xi}$ to obtain

$$v(1 + A \xi) = -\xi \frac{dv}{d \xi} \quad (D8)$$

By the method of separation of variables, both sides of Eq. (D8) are integrated to obtain

$$-\ln(v) = \ln(\xi) + A \xi + c_1 \Rightarrow \frac{d \langle P \rangle}{d \xi} = \frac{c_1}{\xi} e^{(-A \xi)} \quad (D9)$$

The solution to the ordinary differential equation (ODE), Eq. (D9) is

$$\langle P \rangle = c_1 Ei(-A \xi) + c_2 \quad (D10)$$

where c_1 and c_2 are constants of integration.

The boundary conditions, Eq. (42) are introduced to determine c_1 and c_2 , which yield the particular solution for the diffusivity Eq. (D6) as

$$\langle P \rangle = -\frac{1}{\Lambda(0)} e^{(A D_0)} Ei(-A \xi) + P_e \quad (D11)$$

Appendix E. Total mobility in two phase region and impedance calculation

The sum of the overall gas and water velocities, Eq. (B1) results to

$$2\pi r U = Q = - \left[\int_0^H \frac{k(z) k_{rw}(s) dz}{\mu_w} + \int_0^H \frac{k(z) k_{rg}(s) dz}{\mu_g [1 + \beta \Delta \sigma_{cr}(s)]} \right] 2\pi r \frac{\partial p_w}{\partial r} - \int_0^H \frac{k(z) k_{rg}(s) dz}{\mu_g [1 + \beta \Delta \sigma_{cr}(s)]} 2\pi r \frac{\partial p_c(s)}{\partial r} \quad (E1)$$

Substituting the dimensionless parameters Eq. (B3) into Eq. (E1) gives

$$1 = - \left[\int_0^1 K(Z) k_{rw}(s) dZ + \int_0^1 \frac{K(Z) k_{rg}(s) dZ}{\mu [1 + \beta \Delta \sigma_{cr}(s)]} \right] x \frac{\partial P_w}{\partial x} - \delta \int_0^1 \frac{K(Z) k_{rg}(s) dZ}{\mu [1 + \beta \Delta \sigma_{cr}(s)]} x \frac{\partial J(s)}{\partial x} \quad (E2)$$

At large-scale approximations, $\delta \ll 1$, hence the pressure drop in gas and water are equal, that is,

$$\frac{\partial P_g}{\partial x} = \frac{\partial P_w}{\partial x} = \frac{\partial P}{\partial x} \quad (E3)$$

Hence, Eq. (E2) for total flux simplifies to

$$1 = - \left[\int_0^1 K(Z) k_{rw}(s) dZ + \int_0^1 \frac{K(Z) k_{rg}(s) dZ}{\mu [1 + \beta \Delta \sigma_{cr}(s)]} \right] x \frac{\partial P}{\partial x} \quad (E4)$$

The total mobility for all the three zones (0, 01, and 1) defined by Eq. (45) are determined by the following expression.

For zone 0 the total mobility is expressed as

$$\Lambda_0(S) = \int_{Z_0}^1 \frac{K(Z)k_{rg}(s)dZ}{\mu[1 + \beta\Delta\sigma_{cr}(s)]} + \int_0^{Z_0} K(Z)dZ \quad (E5)$$

In zone 01 we obtain

$$\Lambda_{01}(S) = \int_0^{Z_0} K(Z)dZ + \int_{Z_0}^{Z_0+h_c} k_{rw}(s)K(Z)dZ + \int_{Z_0}^{Z_0+h_c} \frac{K(Z)k_{rg}(s)dZ}{\mu[1 + \beta\Delta\sigma_{cr}(s)]} + \frac{k_{rgwc}}{\mu[1 + \beta\Delta\sigma_{cr}]} \int_{Z_0+h_c}^1 K(Z)dZ \quad (E6)$$

Finally, for zone 1, the expression for the total mobility becomes

$$\Lambda_1(S) = \frac{k_{rgwc}}{\mu[1 + \beta\Delta\sigma_{cr}]} \int_{Z_0+h_c}^1 K(Z)dZ + \int_0^{Z_1} \left(k_{rw}(s)K(Z) + \frac{K(Z)k_{rg}(s)}{\mu[1 + \beta\Delta\sigma_{cr}(s)]} \right) dZ \quad (E7)$$

Data availability

No data was used for the research described in the article.

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