

Abrupt-Interface Solution for Carbon Dioxide Injection into Porous Media

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Abstract We derive an approximate analytical solution, which describes the interface dynamics during the injection of supercritical carbon dioxide into homogeneous geologic media that are fully saturated with a host fluid. The host fluid can be either heavier (e.g., brine) or lighter (e.g., methane) than the injected carbon dioxide. Our solution relies on the Dupuit approximation and explicitly accounts for the buoyancy effects. The general approach is applicable to a variety of phenomena involving variable-density flows in porous media. In three dimensions under radial symmetry, the solution describes carbon dioxide injection; its two-dimensional counterpart can be used to model seawater intrusion into coastal aquifers. We conclude by comparing our solutions with existing analytical alternatives.

Keywords Two-phase flow · Sharp interface · CO₂ · Analytical solution

1 Introduction

Sequestration of supercritical carbon dioxide (CO₂) in geological formations is one of the approaches to mitigating the effects of global warming. While possible geological settings are many (e.g., salt formations, depleted oil and gas reservoirs, saline aquifers, coal beds, and deep-sea sediments) (Bachu 2000; House et al. 2006), there exists a general consensus as to the means of delivering CO₂ into the subsurface. Injection wells are used to accomplish this task, which results in complex variable-density flow regimes.

While subsurface flow induced by injection/pumping wells has been studied in detail by groundwater hydrologists and petroleum engineers, modeling of CO₂ injection poses a set

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of unique challenges. These have been the subject of recent numerical (Pruess et al. 2003; Doughty and Pruess 2004) and analytical (Saripalli and McGrail 2002; Riaz et al. 2006; Nordbotten and Celia 2006) studies. The attraction of numerical solutions lies in their versatility and ability to handle complex geochemical processes and various geologic settings. Analytical solutions are invaluable for gaining physical insight into the phenomenon and obtaining quick, back-of-the-envelope calculations of the subsurface capacity for CO₂ storage. They are also used in system-wide assessment and management of subsurface systems (Pawar et al. 2006; Zhang et al. 2007).

Injection of carbon dioxide into a subsurface environment induces nearly immiscible flow of the ambient fluid and supercritical CO₂. The difference between the densities of the two fluids causes their stratification, with the invading CO₂ laying either above or below the host fluid. The first scenario is realized when CO₂ is injected into deep saline aquifers replacing water that is more dense than CO₂; the second scenario occurs when CO₂ is injected into coal beds replacing methane that is less dense than CO₂. Regardless of the injection conditions, the resulting flow regime is substantially different from the so-called plug flow that is predicted by a one-dimensional radial flow model (Pruess et al. 2003).

Proper understanding of the flow dynamics, including the ability to model the shape and evolution of the interface between CO₂ and the host fluid, is the key to addressing a host of practical questions. The larger the surface area of this interface, the more extensive are the geochemical reactions affecting CO₂ and the more successful its long-term storage in the subsurface is likely to be. A quantitative analysis of the dynamics of the interface separating CO₂ and the host fluid is our main goal.

This goal can be accomplished by employing one of the following two modeling approaches. The first relies on two-phase flow equations and yields a diffusive interfacial region wherein the CO₂ saturation S_{CO_2} gradually decreases from $S_{\text{CO}_2} = 1$ in the region fully occupied by the invading CO₂ to $S_{\text{CO}_2} = 0$ in the region that is fully occupied by the host fluid. The second approach, which we pursue here, approximates the interfacial region by an abrupt interface. This approximation is valid as long as flow velocity is high.

We start by describing alternative formulations of the abrupt-interface model in Sect. 2 and presenting an equation describing the interface dynamics under the Dupuit assumption in Sect. 3. We proceed by deriving closed-form analytical solutions that describe the two- (Sect. 4.1) and three-dimensional (Sect. 4.2) interface dynamics for CO₂ injected into homogeneous geologic media occupied alternatively by a heavier (e.g., saline water) or lighter (e.g., methane) host fluid. In Sect. 4.3, we contrast these solutions with their semi-analytical counterparts obtained by Nordbotten et al. (2005) and Nordbotten and Celia (2006).

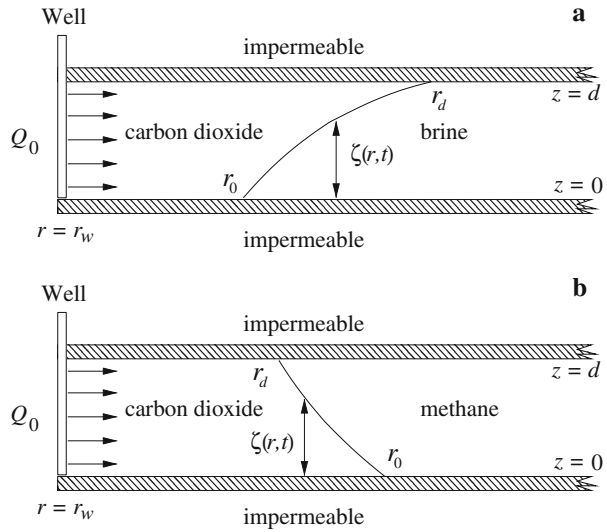
2 Problem Formulation

Consider injection of CO₂ from a fully penetrating well of radius r_w into a deep confined aquifer of thickness d (see Fig. 1). For standard operating conditions, CO₂ remains supercritical and in thermal equilibrium with the host fluid (Bachu 2003; Nordbotten et al. 2005, and references therein). Macroscopic fluxes \mathbf{q}_i of CO₂ ($i = c$) and host fluid ($i = w$) satisfy Darcy's law

$$\mathbf{q}_i = -\frac{kk_i \rho_i g}{\mu_i} \nabla h_i, \quad i = c, w, \quad (1)$$

where ρ_i and μ_i are the density and viscosity of the i -th fluid, g is gravity acceleration, k is the intrinsic permeability of the medium, and k_i is the saturation-dependent relative permeability

Fig. 1 A schematic representation of supercritical CO₂ injection into a porous medium occupied by (a) a heavier or (b) a lighter host fluid. The invading CO₂ and the host fluid are separated by the abrupt interface $\zeta(r, t)$



of the medium for the i -th fluid. The hydraulic head h_i in each phase is given in terms of pressure p_i as

$$h_i = \frac{p_i}{\rho_i g} + z, \tag{2}$$

where z is the vertical coordinate. A two-phase formulation of the problem is completed by combining (1) with mass conservation equations for the two fluids and specifying empirical constitutive relations between relative permeability and saturation and between saturation and capillary pressure between the two fluids. Doughty and Pruess (2004) used a similar formulation to numerically model the injection of supercritical CO₂ into the subsurface.

Numerical analyses of multi-phase flow are notoriously challenging and prone to errors. Instead, we employ an abrupt-interface approximation, which stipulates the existence of an interface separating a region saturated with the host fluid from a region occupied by the advancing CO₂. While an abrupt interface between immiscible (or miscible) fluids cannot exist in a macroscopic (Darcian) sense, in many situations of practical interest the transition zone between two (miscible) fluids is relatively narrow or the (immiscible) displacement is almost complete, so that the approximation of an abrupt interface separating the two fluids is justified (Bear 1972, p. 439).

The abrupt-interface approximation is generally valid for flow regimes with a large Péclet number, a condition that is expected to hold during CO₂ injection. This abrupt-interface approximation has been used to analyze various multi-phase flow phenomena in porous media (Bear 1972), including CO₂ sequestration Nordbotten et al. (2005), Nordbotten and Celia (2006). For a certain range of density and viscosity ratios, the moving front can become unstable. An important question of the stability of CO₂ fronts displacing a host fluid lies outside the scope of the present analysis.

From the outset, it is important to recognize the fundamental differences between the abrupt-interface approximation and the Buckley-Leverett approximation (Buckley and Leverett 1942). Both approaches assume that capillary pressure is constant and are widely used in analytical analyses of multiphase flow in porous media. However, the Buckley-Leverett approximation allows for saturation variability behind the displacement front (i.e.,

it accounts for the dependence of permeability on saturation), but ignores buoyancy effects (Bear 1972, p. 468). The abrupt-interface solution we develop explicitly incorporates buoyancy effects but disregards saturation variability. Thus, the two approaches are complementary.

Within the abrupt-interface framework, a quasi-steady (successive steady-states) description of moving fronts is obtained by combining the Darcian fluxes \mathbf{q}_i in (1) with continuity equations (Bear 1972, p. 566)

$$\nabla \cdot \mathbf{q}_i = 0, \quad i = c, w. \tag{3}$$

Let $Q_0(t)$ denote the volumetric flux of the injected CO_2 , and $\zeta(r, t)$ denote the vertical position of the resulting interface between CO_2 and water (Fig. 1). Setting the time at which the injection commenced to $t = 0$, the total volume of CO_2 injected into the porous medium at time t is given by

$$V(t) = \int_0^t Q_0(t') dt' = \phi \int_{\Omega_c} dx, \tag{4}$$

where ϕ is the porosity of the medium, and Ω_c is the part of the medium occupied by CO_2 . The second equality is the consequence of the incompressibility of both fluids in the absence of internal sources and sinks, and assumes that the pores in Ω_c are completely occupied with CO_2 . In general, the pores in Ω_c can contain the trapped host fluid with a residual saturation S_r . This phenomenon can be accounted for by replacing the porosity ϕ with the drainable porosity $\phi_d \equiv (1 - S_r)\phi$ (Bear 1972, p. 88).

3 Interface Dynamics

An analytical treatment of the CO_2 injection is facilitated by realization of mathematical similarities between this problem and that of saltwater intrusion into coastal aquifers. The latter problem has been the subject of numerous analytical studies (Bear 1972).

Integrating (3) over the aquifer thickness yields

$$\nabla^h \cdot \int_0^\zeta \mathbf{q}_w^h dz - \nabla^h \zeta \cdot \mathbf{q}_w^h(z = \zeta) + q_{wz}(z = \zeta) - q_{wz}(z = 0) = 0, \tag{5}$$

where ζ is the interface height; ∇ is the nabla operator; and the superscript h denotes the horizontal component of the vectors ∇ and \mathbf{q}_w , with q_{wz} representing the vertical component of the latter. The vertical velocity at the interface is given by

$$q_{wz}(z = \zeta) = \phi \frac{d\zeta}{dt} = \phi \frac{\partial \zeta}{\partial t} + \nabla^h \zeta \cdot \mathbf{q}_w^h(z = \zeta). \tag{6}$$

Combining (5) and (6), while assuming that the top and bottom boundaries are impermeable, i.e., $q_{wz}(z = 0) = 0$, leads to a flow equation for the water phase,

$$\nabla^h \cdot \mathbf{Q}_w^h + \phi \frac{\partial \zeta}{\partial t} = 0, \quad \mathbf{Q}_w^h \equiv \int_0^\zeta \mathbf{q}_w^h dz. \tag{7}$$

With the same reasoning, we obtain for the CO₂ phase

$$\nabla^h \cdot \mathbf{Q}_c^h + \phi \frac{\partial(d - \zeta)}{\partial t} = 0. \tag{8}$$

Equations (7) and (8) imply that in the absence of other sources, $\mathbf{Q}_0^h = \mathbf{Q}_c^h + \mathbf{Q}_w^h$ is divergence-free

$$\nabla^h \cdot \mathbf{Q}_0^h = 0. \tag{9}$$

Employing the Dupuit assumption of horizontal flow yields

$$\mathbf{Q}_w^h = \zeta \mathbf{q}_w^h, \quad \mathbf{Q}_c^h = (d - \zeta) \mathbf{q}_c^h. \tag{10}$$

The horizontal Darcian fluxes \mathbf{q}_w^h and \mathbf{q}_c^h are obtained from (1) by setting the two relative permeabilities $k_i = 1$ ($i = c, w$), which gives

$$\mathbf{Q}_w^h = -\zeta \frac{k \rho_w g}{\mu_w} \nabla^h h_w, \quad \mathbf{Q}_c^h = -(d - \zeta) \frac{k \rho_c g}{\mu_c} \nabla^h h_c. \tag{11}$$

Setting $k_i = 1$ ($i = c, w$) implies that the advancing interface separates the regions of a porous medium where saturations of CO₂ are 1 (behind the front) and 0 (ahead of the front). In order to account for the presence of the host fluid trapped behind the advancing CO₂ front, i.e., for the residual saturation $S_r \neq 0$, one should replace μ_c with μ_c/k_c^* in (11) and below. Here, k_c^* is the relative permeability for CO₂ evaluated at the residual saturation S_r .

According to (2), the condition $p_c = p_w$ at the interface $z = \zeta$ implies that

$$\zeta = \frac{\rho_w h_w - \rho_c h_c}{\rho_w - \rho_c}. \tag{12}$$

By partial differentiation, we obtain

$$\nabla^h \zeta = \pm \left[\frac{\rho_w}{\Delta \rho} \nabla^h h_w - \frac{\rho_c}{\Delta \rho} \nabla^h h_c \right], \quad \Delta \rho \equiv \rho_w - \rho_c. \tag{13}$$

Note that for a lighter fluid displacing a heavier fluid, the slope of the interface is positive, and vice versa. Thus, the plus sign in (13) corresponds to the injection scenario in which a lighter fluid displaces a heavier fluid (Fig. 1a). Injection under the opposite conditions (Fig. 1b) is described by the minus sign. Combining (7)–(13), we obtain

$$\nabla^h \cdot \left[\zeta \frac{\mathbf{Q}_0^h \pm \Delta \rho \frac{k}{\mu_c} (d - \zeta) \nabla^h \zeta}{\zeta + \lambda(d - \zeta)} \right] + \phi \frac{\partial \zeta}{\partial t} = 0, \tag{14}$$

where $\lambda = \mu_w/\mu_c$ is the viscosity ratio. The derivation of exact analytical solutions to this nonlinear equation for interface displacement was deemed impossible (Bear 1972, p. 535). One of our goals is to obtain approximate analytical solutions of (14). Another goal is to contrast these solutions with those obtained with the variational approach of Nordbotten et al. (2005). The latter goal is accomplished in Sect. 4.3.

4 Analytical Solutions

The analytical solutions derived in this section rely on the Dupuit assumption of predominantly horizontal flow, and are similar in spirit to the Ghyben-Herzberg solution for static interface position in seawater intrusion problems (Bear 1972, Sects. 9.7.2 and 9.7.3). We start

by deriving in Sect. 4.1 an approximate solution for interface dynamics in two spatial dimensions, which is of direct relevance to seawater intrusion. In Sect. 4.2, we derive a solution for three-dimensional flow in radial coordinates, which can be used to model CO₂ injection. Section 4.3 contains a comparison of our solutions with those obtained via the variational approach of Nordbotten et al. (2005).

4.1 Two Dimensions

Consider two-dimensional planar flow in a homogeneous porous medium, as shown in Fig. 1, wherein r is to be replaced with x . We set the width of the injection interval to $r_w \equiv x_w = 0$ and denote the trailing edge of the moving interface by $x_0(t)$. The Darcy equations (1) for each fluid i under the Dupuit assumption read as

$$q_{i1}(x) = -\frac{k\rho_i g}{\mu_i} \frac{dh_i(x)}{dx}. \tag{15}$$

A two-dimensional version of (13) is given by

$$\frac{d\zeta(x)}{dx} = \pm \left| \frac{dh_w(x)}{dx} \frac{\rho_w}{\Delta\rho} - \frac{dh_c(x)}{dx} \frac{\rho_c}{\Delta\rho} \right|. \tag{16}$$

Substituting (15) into (16) yields

$$\frac{d\zeta(x)}{dx} = \pm \left| \frac{\mu_w q_{wx}(x) - \mu_c q_{cx}(x)}{\Delta\rho k} \right|. \tag{17}$$

The total volumetric fluxes of water and CO₂ in (11) are given by

$$Q_w(x, t) = \zeta q_{w1}, \quad Q_c(x, t) = (d - \zeta)q_{c1}. \tag{18}$$

At the same time, the total volumetric fluxes of CO₂ and water are given by the proportion of the total volumetric flux that corresponds to the fraction of the medium cross-section occupied by the respective fluid, i.e.,

$$Q_w(x, t) = \frac{\zeta}{d} Q_0(t), \quad Q_c(x, t) = \frac{d - \zeta}{d} Q_0(t). \tag{19}$$

Comparison of (18) and (19) reveals that the Darcy velocities are constant,

$$q_{w1}(x) = q_{c1}(x) = \frac{Q_0}{d}. \tag{20}$$

The subsequent derivations use the plus sign in (17), which corresponds to injection of CO₂ (a lighter fluid) into a brine (a heavier fluid) formation. Substituting (20) into (17) and integrating from $x_0(t)$ to x , we obtain an expression for the interface dynamics

$$\zeta(x) = \gamma_{cw}^{(2d)}(x - x_0) \quad \text{or} \quad x(\zeta) = \frac{\zeta}{\gamma_{cw}^{(2d)}} + x_0. \tag{21}$$

The dimensionless group $\gamma_{cw}^{(2d)}$, which is defined by

$$\gamma_{cw}^{(2d)} = \frac{Q_0 \Delta\mu}{kdg \Delta\rho}, \quad \Delta\mu = \mu_w - \mu_c, \tag{22}$$

quantifies the relative importance of viscous, gravity, and pressure forces. It follows from (4) and (21) that the total injected volume of CO₂ is

$$\frac{V(t)}{\phi} = \int_0^d x(\zeta) d\zeta = \frac{d^2}{2\gamma_{cw}^{(2d)}} + x_0(t)d. \tag{23}$$

This allows one to determine the position of the trailing edge of the interface, $x_0(t)$, as

$$x_0(t) = \frac{V(t)}{\phi d} - \frac{d}{2\gamma_{cw}^{(2d)}}. \tag{24}$$

Substituting (24) into the first expression in (21) yields the final expression for the interface dynamics

$$\zeta(x, t) = \gamma_{cw}^{(2d)} \left[x - \frac{V(t)}{\phi d} \right] + \frac{d}{2}, \quad x \geq x_0(t). \tag{25}$$

Equation (25) is a traveling wave solution of the general equation (14), which hitherto had to be solved numerically (Bear 1972, p. 535). It predicts that the interface separating the two fluids is a straight line. The slope of this straight line depends on the relative importance of viscous, gravity, and pressure forces, as quantified by the dimensionless parameter $\gamma_{cw}^{(2d)}$.

4.2 Three Dimensions

In three dimensions, we consider a radially symmetric injection scenario. Under the Dupuit assumption, the hydraulic head in each phase depends only on the radial coordinate, $h_i(\mathbf{x}) = h_i(r)$. For the i -th phase ($i = w, c$), the Darcy equation (1) yields in radial coordinates

$$q_{ir} = -\frac{k\rho_i g}{\mu_i} \frac{dh_i(r)}{dr}, \quad i = w, c. \tag{26}$$

In radial coordinates, (13) takes the form

$$\frac{d\zeta(r)}{dr} = \pm \left| \frac{dh_w(r)}{dr} \frac{\rho_w}{\Delta\rho} - \frac{dh_c(r)}{dr} \frac{\rho_c}{\Delta\rho} \right|. \tag{27}$$

For a lighter fluid displacing a heavier fluid, the slope of the interface is positive, and vice versa. Substituting (26) into (27) yields

$$\frac{d\zeta(r)}{dr} = \pm \left| \frac{1}{\Delta\rho k g} [\mu_w q_{wr}(r) - \mu_c q_{cr}(r)] \right|. \tag{28}$$

The Dupuit assumption suggests that the radial Darcy velocities do not depend on the vertical position, and therefore the total fluxes of the respective fluids are given by

$$Q_w(r, t) = 2\pi r \zeta q_{wr}, \quad Q_c(r, t) = 2\pi r (d - \zeta) q_{cr}. \tag{29}$$

At the same time, the total volumetric fluxes of CO₂ and water are given by the proportion of the total volumetric flux that corresponds to the fraction of the medium cross-section occupied by the respective fluid, i.e.,

$$Q_w(r, t) = \frac{\zeta}{d} Q_0(t), \quad Q_c(r, t) = \frac{d - \zeta}{d} Q_0(t). \tag{30}$$

Combining (29) and (30) gives

$$q_{wr}(r) = q_{cr}(r) = \frac{Q_0}{2\pi rd}. \tag{31}$$

Substituting (31) into (28) and integrating from r_0 to r yields

$$\zeta(r, t) = d\gamma_{cw} \ln \left[\frac{r}{r_0(t)} \right], \quad \gamma_{cw} = \frac{Q_0}{2\pi kd^2g} \frac{\Delta\mu}{\Delta\rho}. \tag{32}$$

In order to find the radius r_d at which the interface intersects the upper domain boundary, we set $\zeta = d$ in (32). This gives

$$r_d = r_0 \exp(1/\gamma_{cw}). \tag{33}$$

We obtain the radius r_0 from mass conservation using (4). To this end, we invert (32), which yields

$$r = r_0 \exp \left(\frac{\zeta}{d\gamma_{cw}} \right). \tag{34}$$

Substituting (34) into the second integral in (4) and recalling that $r_0 \gg r_w$, we obtain

$$V(t) = \pi \int_0^d r^2 d\zeta = r_0^2 \frac{\pi\phi d\gamma_{cw}}{2} \left[\exp \left(\frac{2}{\gamma_{cw}} \right) - 1 \right] \tag{35}$$

or

$$r_0(t) = \sqrt{\frac{2V_0(t)}{\pi\phi d\gamma_{cw}} \left[\exp \left(\frac{2}{\gamma_{cw}} \right) - 1 \right]^{-1}}. \tag{36}$$

For a constant total volumetric flux, the total injected volume is given by $V_0(t) = Q_0t$, which implies that the interface propagates as $r_0(t) \sim \sqrt{t}$.

Inserting (36) into (32) and defining the dimensionless height and radius as

$$\zeta' \equiv \frac{\zeta}{d}, \quad r' \equiv r \sqrt{\frac{\pi\phi d}{V_0(t)}}, \tag{37}$$

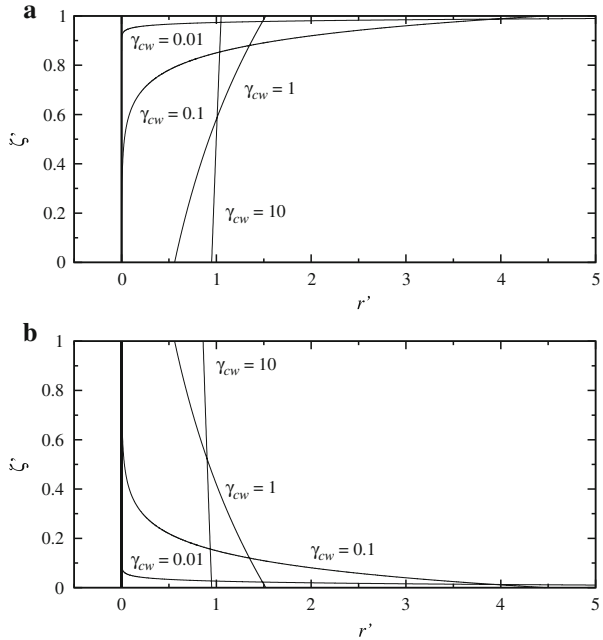
respectively, (32) can be written in a dimensionless form as

$$\zeta'(r') = \gamma_{cw} \ln \left[r' \sqrt{\frac{\gamma_{cw}}{2}} (e^{2/\gamma_{cw}} - 1) \right]. \tag{38}$$

We consider the limits of small and large γ_{cw} in (32). This parameter accounts for both the difference between the physical properties of two fluids (their densities and viscosities) and the injection rate relative to the formation conductivity. Small γ_{cw} corresponds to flow regimes in which gravity forces dominate viscous forces and large γ_{cw} vice versa. In order to derive an approximation for $\zeta'(r')$ for $|\gamma_{cw}| \ll 1$, we rewrite (38) as

$$\zeta'(r') = \gamma_{cw} \left\{ \ln(r') + \frac{1}{2} \ln \left[\frac{\gamma_{cw}}{2} (e^{2/\gamma_{cw}} - 1) \right] \right\}. \tag{39}$$

Fig. 2 Interfaces predicted by (38) for (a) $\gamma_{cw} = 10^{-2}, 10^{-1}, 1$ and 10, i.e., for a less dense fluid injected into a denser fluid and (b) for $\gamma_{cw} = -10^{-2}, -10^{-1}, -1$ and -10 , i.e., for a denser fluid injected into a less dense one



The expansion of the last term depends on the sign of γ_{cw} . For small $|\gamma_{cw}| \ll 1$, the dimensionless interface position (32) can be approximated by

$$\zeta'(r') = \begin{cases} 1 + \frac{\gamma_{cw}}{2} [2 \ln(r') + \ln(\gamma_{cw}) - \ln(2)] + \dots, & \gamma_{cw} > 0 \\ \frac{\gamma_{cw}}{2} [2 \ln(r') + \ln(|\gamma_{cw}|) - \ln(2)] + \dots, & \gamma_{cw} < 0 \end{cases} \tag{40}$$

where the dots indicate subleading contributions that decrease exponentially fast as γ_{cw} tends to zero. Expression (40) describes the spreading of a thin layer of CO₂ on top/bottom of the denser/less dense fluid.

For large $|\gamma_{cw}| \gg 1$, (38) reduces to $\zeta' = \gamma_{cw} \ln(r')$. Since ζ' must be positive, r' must be greater than 1. This yields

$$\zeta'(r') = \mathcal{H}(r' - 1), \tag{41}$$

where $\mathcal{H}(\cdot)$ is the Heaviside function defined as $\mathcal{H}(a) = 1$ for $a \geq 0$ and $\mathcal{H}(a) = 0$ for $a < 0$. Equation (41) demonstrates that, for injection regimes with $|\gamma_{cw}| \gg 1$, the CO₂ front advances as a vertical plug.

Figure 2 illustrates the shapes of the CO₂-host fluid interface computed with (38) for several values of the dimensionless parameter γ_{cw} . Since the dimensionless radius r' in (37) is time-dependent, this figure also describes the interface dynamic. For large values of $|\gamma_{cw}|$, the interface shape is close to the vertical line $r' = 1$, which is consistent with the plug flow predicted by the asymptotic solution (41).

As $\gamma_{cw} > 0$ decreases, the trailing edge of the interface $r_0(t)$ recedes towards the well, while its leading edge $r_d(t)$ moves further ahead, and the interface becomes more convex

(Fig. 2a). For sufficiently small $\gamma_{cw} > 0$, CO_2 advances as a horizontal layer located at the top of the flow domain.

For negative γ_{cw} , the situation is reversed (Fig. 2b). As $\gamma_{cw} < 0$ decreases, $r_0(t)$ advances further inside the flow domain, while $r_d(t)$ trails behind; the interface becomes more concave. For sufficiently small $\gamma_{cw} \ll -1$, CO_2 advances as a horizontal layer located at the bottom of the flow domain.

It is worthwhile recalling that the positive and negative γ_{cw} s correspond to the two injection scenarios shown in Figs. 1a and 1b, respectively. Positive values of γ_{cw} imply the injection of CO_2 into a formation occupied by a heavier host fluid, and negative values indicate that the host fluid is lighter.

4.3 Comparison with Variational Solutions

The solutions described above explicitly incorporate the buoyancy effects but rely on the Dupuit approximation. The semi-analytical variational solution of Nordbotten et al. (2005) does not explicitly invoke the Dupuit approximation but accounts for the buoyancy effects indirectly. This is done by postulating that the injected body of CO_2 advances in a way that minimizes its potential energy. In this section, we compare our solutions with their variational counterparts and examine the validity of the minimum energy postulate.

4.3.1 Three Dimensions

Rewriting (14) in radial coordinates, disregarding gravity (i.e., setting $\Delta\rho = 0$), and rescaling ζ and r according to (37) gives,

$$\frac{1}{r'} \frac{\partial}{\partial r'} \frac{\zeta'}{\zeta'(1-\lambda) + \lambda} + t \frac{\partial \zeta'}{\partial t} + r' \frac{\partial \zeta'}{\partial r'} = 0. \tag{42}$$

This is similar to Eq. 11 of Nordbotten and Celia (2006) wherein gravity is disregarded (note that we rescale r differently). Equation (42) has the following stationary solution

$$\zeta'(r') = \frac{\lambda}{\lambda - 1} \left(1 - \frac{1}{r' \sqrt{\lambda}} \right), \tag{43}$$

which was also obtained by Nordbotten et al. (2005) using a variational approach.

In order to include buoyancy, Nordbotten et al. (2005) postulate that the interface $\zeta'(r', t)$ takes the shape, which minimizes “the energy required to submerge the lighter CO_2 into the denser water” (see the following section for a detailed implementation of this approach to two-dimensional flow). The resulting variational analysis yields a solution for the interface, whose shape is defined as a real root of an algebraic equation

$$-\frac{\lambda - 1}{r' [\lambda - \zeta'(\lambda - 1)]^2} + 2\Gamma r'(1 - \zeta') + 2\Lambda r' = 0. \tag{44}$$

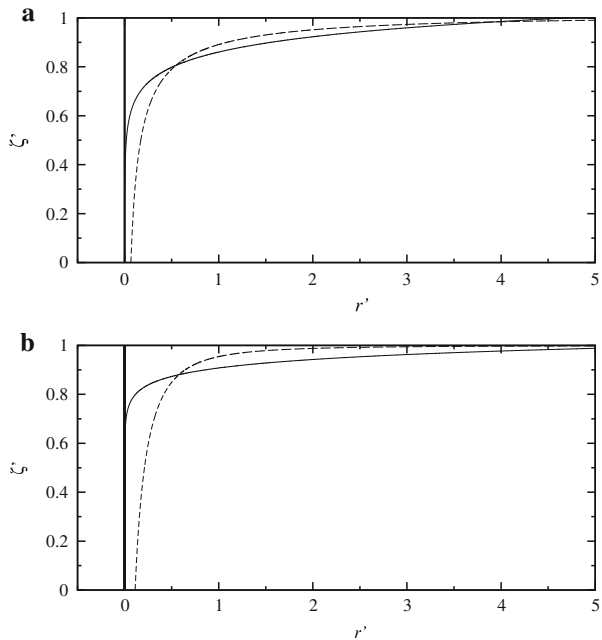
Here, the Lagrange multiplier Λ is given by a solution of the transcendental equation

$$(\lambda - 1)\Lambda + \frac{\lambda\Gamma}{\lambda - 1} \ln \left(\frac{\Gamma + \Lambda}{\Lambda\lambda} \right) - 2\lambda \left(\Lambda - \frac{\Gamma}{\lambda - 1} \right)^2 = \Gamma, \tag{45}$$

and the dimensionless group Γ is defined by

$$\Gamma = \frac{2\pi k d^2 g \Delta\rho}{Q_0}. \tag{46}$$

Fig. 3 Interfaces calculated using Eq. 38 (solid lines) and with the variation scheme of Nordbotten et al. (2005) (dashed lines) for $\Gamma = 10$; (a) $\lambda = 2$ and (b) $\lambda = 10$



For $\Gamma = 0$ (i.e., $\Delta\rho = 0$), the solution of (44) and (45) reduces to (43).

Figure 3 compares our analytical solution (38) with numerical solutions of (44)–(46) for a buoyancy-dominated scenario with $\Gamma = 10$, and $\lambda = 2$ and 10. The solutions are qualitatively similar, with (38) predicting the trailing edge closer to and the leading edge further away from the injection well. Solution (38) predicts more mass at the top of the domain than the variational approach.

In order to understand the quantitative differences between the two approaches, we apply the variational approach of Nordbotten et al. (2005) to a two-dimensional injection scenario. This allows us to elucidate the veracity of the minimum energy postulate.

4.3.2 Two Dimensions

We now consider CO₂ injection into a two-dimensional semi-infinite aquifer employing the variation approach of Nordbotten et al. (2005). Average pressure \bar{p} satisfies the flow equation

$$-k \frac{\partial}{\partial x} \lambda^* \frac{\partial}{\partial x} \bar{p} = \frac{1}{d} Q_0 \delta(x - x_w), \tag{47}$$

where λ^* is defined by

$$\lambda^* = \frac{b}{\mu_c d} + \frac{d - b}{\mu_w d}. \tag{48}$$

The interface elevation is $\zeta = d - b(x)$. A solution of (47) is given by

$$p(x_w) - p(x_d) = \frac{Q_0 \mu_w}{kd} \int_{x_w}^{x_d} \frac{dx'}{(\lambda - 1)b + d}. \tag{49}$$

The (potential) energy needed to submerge lighter CO₂ into denser brine can be expressed as

$$\Delta E_p = \frac{Q_0}{V(t)} \int_0^d \Delta \rho g b x(b) db. \tag{50}$$

The dimensionless energy functional $E\{x(b)\}$ is obtained by combining (50) with the volume work associated with the injection by pressure (49) and the volume constraint

$$V(t) = \phi \int_0^1 x(b) db. \tag{51}$$

After rescaling and change of variables, one obtains

$$E\{x(b)\} = - \int_0^1 \frac{(\lambda - 1)x(b')db'}{[(\lambda - 1)b' + 1]^2} + \Gamma \int_0^1 b'x(b')db' + \Lambda \int_0^1 x(b')db'. \tag{52}$$

Since the boundary terms independent of $x(\zeta)$ do not contribute to the variation, they are suppressed here for simplicity. Variation of (52) with respect to $x(b)$ leads to

$$- \frac{\lambda - 1}{[\lambda - (\lambda - 1)\zeta]^2} + \Gamma\zeta + \Lambda = 0, \tag{53}$$

which implies that the elevation $\zeta = 1 - b$ of the interface does not depend on x .

This can occur either if the interface is horizontal or vertical. The former requires an infinite amount of injected CO₂, and is thus unphysical. Thus, the vertical interface, i.e., plug flow, is the only possible outcome of the energy optimization approach. Such a behavior is likewise unphysical, since the CO₂ front is expected to advance further into the top of aquifer than its bottom, as predicted by our solution (25). This leads one to conclude that the minimum energy postulate is not valid in two dimensions. This finding suggests that it is also invalid in three dimensions.

5 Summary and Conclusions

We derived closed-form analytical solutions describing the dynamics of interfaces in two- and three-dimensional porous media. A typical interface separates two fluids with different physical properties, i.e., density and viscosity. Examples include seawater intrusion in coastal aquifers, where an interface separates saline and fresh groundwater, and carbon dioxide sequestration in the subsurface, wherein CO₂ is injected into a deep aquifer. Our two-dimensional solution describes the former phenomenon, while its three-dimensional counterpart models the latter. The solutions hold either when a less dense fluid is introduced into a porous medium occupied by a denser fluid or when the situation is reversed. For the solutions to remain valid, flow has to reach a quasi-steady regime after the initial injection phase, and the Dupuit approximation has to be valid.

Our analysis leads to the following major conclusions.

1. Two-dimensional flow regimes are characterized by a linear interface, whose slope is determined by a single dimensionless parameter that accounts for the viscosity and density contrasts of the two fluids.

2. Three-dimensional flow regimes are characterized by a logarithmic interface, whose curvature is controlled by a single dimensionless parameter that compares the relative strength of viscous and buoyancy forces.
3. Our two-dimensional analysis casts doubt on the validity of the postulate that the injected body of CO₂ advances in a way that minimizes its potential energy.

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References

- Bachu, S.: Sequestration of CO₂ in geological media: criteria and approach for site selection in response to climate change. *Energy Convers. Manage.* **41**(9), 953–970 (2000)
- Bachu, S.: Screening and ranking of sedimentary basins for sequestration of CO₂ in geological media. *Environ. Geol.* **44**(3), 277–289 (2003)
- Bear, J.: *Dynamics of Fluids in Porous Media*. Elsevier, New York (1972)
- Buckley, S.E., Leverett, M.C.: Mechanism of fluid displacements in sands. *Trans. AIME* **146**, 107–116 (1942)
- Doughty, C., Pruess, K.: Modeling supercritical carbon dioxide injection in heterogeneous porous media. *Vadose Zone J.* **3**, 837–847 (2004)
- House, K.Z., Schrag, D.P., Harvey, C.F., Lackner, K.S.: Permanent carbon dioxide storage in deep-sea sediments. *Proc. Natl. Acad. Sci. USA* **103**(33), 12291–12295 (2006)
- Nordbotten, J.M., Celia, M.A.: Similarity solutions for fluid injection into confined aquifers. *J. Fluid Mech.* **561**, 307–327 (2006)
- Nordbotten, J.M., Celia, M.A., Bachu, S.: Injection and storage of CO₂ in deep saline aquifers: Analytical solution for CO₂ plume evolution during injection. *Transp. Porous Media* **58**, 339–360 (2005)
- Pawar, R.J., Warpinski, N.R., Lorenz, J.C., Benson, R.D., Grigg, R.B., Stubbs, B.A., Stauffer, P.H., Krumhansl, J.L., Cooper, S.P., Svec, R.K.: Overview of a CO₂ sequestration field test in the West Pearl Queen reservoir, New Mexico. *Environ. Geosci.* **13**(3), 163–180 (2006)
- Pruess, K., Xu, T.F., Apps, J., Garcia, J.: Numerical modeling of aquifer disposal of CO₂. *SPE J.* **8**(1), 49–60 (2003)
- Riaz, A., Hesse, M., Tchelepi, H.A., Orr, F.M. Jr.: Onset of convection in a gravitationally unstable diffusive boundary layer in porous media. *J. Fluid Mech.* **548**, 87–111 (2006)
- Saripalli, P., McGrail, P.: Semi-analytical approaches to modeling deep well injection of CO₂ for geological sequestration. *Energy Convers. Manage.* **43**(2), 185–198 (2002)
- Zhang, Y., Oldenburg, C.M., Finsterle, S., Bodvarsson, G.S.: System-level modeling for economic evaluation of geological CO₂ storage in gas reservoirs. *Energy Convers. Manage.* **48**(6), 1827–1833 (2007)