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A mathematical model of the footprint of the CO₂ plume during and after injection in deep saline aquifer systems

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Abstract

We present a sharp-interface mathematical model of CO₂ migration in saline aquifers, which accounts for gravity override, capillary trapping, natural groundwater flow, and the shape of the plume during the injection period. The model leads to a nonlinear advection–diffusion equation, where the diffusive term is due to buoyancy forces, not physical diffusion. For the case of interest in geological CO₂ storage, in which the mobility ratio is very unfavorable, the mathematical model can be simplified to a hyperbolic equation. We present a complete analytical solution to the hyperbolic model. The main outcome is a closed-form expression that predicts the ultimate footprint on the CO₂ plume, and the time scale required for complete trapping. The capillary trapping coefficient emerges as the key parameter in the assessment of CO₂ storage in saline aquifers. The expressions derived here have immediate applicability to the risk assessment and capacity estimates of CO₂ sequestration at the basin scale. In a companion paper [Szulczewski and Juanes, GHGT-9, Paper 463 (2008)] we apply the model to specific geologic basins.

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1. Introduction

Deep saline aquifers are attractive geological formations for the injection and long-term storage of CO₂ [1]. Even if injected as a supercritical fluid—dense gas—the CO₂ is buoyant with respect to the formation brine. Several trapping mechanisms act to prevent the migration of the buoyant CO₂ back to the surface, and these include [1]: (1) hydrodynamic trapping: the buoyant CO₂ is kept underground by an impermeable cap rock [2]; (2) capillary trapping: disconnection of the CO₂ phase into an immobile (trapped) fraction [3–5]; (3) solution trapping: dissolution of the CO₂ in the brine, possibly enhanced by gravity instabilities [6–7]; and (4) mineral trapping: geochemical binding to the rock due to mineral precipitation [8]. Because the time scales associated with these mechanisms are believed to be quite different ($t_{\text{hydrodyn}} \sim t_{\text{capil}} < t_{\text{dissol}} \ll t_{\text{miner}}$), it is justified to neglect dissolution and mineral trapping in the study of CO₂ migration during the injection and early post-injection periods—precisely when the risk for leakage is higher. During the injection of CO₂ in the geologic formation, the

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gas saturation increases. Once the injection stops, the CO₂ continues to migrate in response to buoyancy and regional groundwater flow. At the leading edge of the CO₂ plume, gas continues to displace water in a drainage process (increasing gas saturation), whilst at the trailing edge water displaces gas in an imbibition process (increasing water saturations). The presence of an imbibition saturation path leads to snap-off at the pore scale and, subsequently, trapping of the gas phase. A trail of residual, immobile CO₂ is left behind the plume as it migrates along the top of the formation [5].

The important questions that we address in this paper are: how far will the CO₂ plume travel (that is, what is the footprint of the plume)?, and for how long does the CO₂ remain mobile? An answer to these questions is essential in any first-order evaluation of the risk of a CO₂ storage project, and for obtaining capacity estimates at the basin scale.

In this paper, we develop a sharp-interface model of CO₂ injection and migration subject to background groundwater flow and capillary trapping. The model is one-dimensional, but captures the gravity override due to the density and mobility contrast between CO₂ and brine. When the mobility contrast is sufficiently high (as it is in the case of interest), we find, by solving the full problem numerically, that the model can be simplified to a hyperbolic equation.

We find a complete analytical solution to the hyperbolic model. This gives a closed-form expression for the footprint of the plume, and the associated time scale for complete immobilization of CO₂ by residual trapping. A capillary trapping coefficient Γ emerges as the key parameter governing the footprint of the CO₂ plume.

2. Description of the Physical Model

A schematic of the basin-scale geologic setting for which the flow model is developed is shown in Figure 1. The CO₂ is injected in a deep formation (blue) that has natural groundwater flow (West to East in the diagram). The injection wells (red) are placed forming a line-drive pattern. Under these conditions, the flow does not have large variations in the North–South direction. This simplification justifies the one-dimensional flow model developed here. We divide the study of the migration of CO₂ into two periods, shown in Figure 2:

1. Injection period. Carbon dioxide (white) is injected at a high flow rate, displacing the brine (deep blue) to its irreducible saturation. Due to buoyancy, the injected CO₂ forms a gravity tongue.
2. Post-injection period. Once injection stops, the CO₂ plume continues to migrate due to its buoyancy and the background hydraulic gradient. At the trailing edge of the plume, CO₂ is trapped in residual form (light blue).

The plume continues to migrate laterally, progressively decreasing its thickness until all the CO₂ is trapped.

Sharp-interface models of gravity currents in porous media have been studied for a long time (see, e.g., [9–10]). Analytical solutions for the evolution of an axisymmetric gravity current have been presented in [11–13] (this last work in the context of CO₂ leakage through abandoned wells). Early-time and late-time similarity solutions for 1D gravity currents in horizontal aquifers are presented in [14]. Of particular relevance is the recent work [15]: they developed a one-dimensional model that includes capillary trapping and aquifer slope (which leads to an advection term). They solved their model numerically and used a “unit square” as the initial shape of the plume after injection.

In the next section we present a sharp-interface mathematical model for the conceptual model of Figure 2. Distinctive features of our model are:

1. We model the injection period. We show that the shape of the plume at the end of injection leads to exacerbated gravity override, which affects the subsequent migration of the plume in a fundamental way.
2. We include the effect of regional groundwater flow, which is essential in the evolution of the plume after injection stops.

3. Mathematical Model

We adopt a sharp-interface approximation [10], by which the medium is assumed to either be filled with water (water saturation $S_w = 1$), or filled with CO₂ (“gas” saturation $S_g = 1 - S_{wc}$, where $S_{wc}$ is the irreducible connate water saturation). We assume that the dimension of the aquifer is much larger horizontally than vertically, so that the vertical flow equilibrium approximation [16], is applicable.

The aquifer is assumed to be horizontal, homogeneous and isotropic. The fluid densities and viscosities are taken as constant. Indeed, compressibility and thermal expansion effects counteract each other, leading to a fairly constant
supercritical CO₂ density over a significant range of depths [17]. We also assume that dissolution into brine and leakage through the caprock are neglected. These assumptions are reviewed critically in the Discussion section.

3.1. Injection Period

Consider the encroachment of the injected CO₂ plume into the aquifer, as shown in Fig. 2(a). The density of the CO₂, ρ, is lower than that of the brine, ρ + Δρ. Let hₙ be the thickness of the (mobile) CO₂ plume, and H the total thickness of the aquifer.

The horizontal volumetric flux of each fluid is calculated by the multiphase flow extension of Darcy’s law, which involves the relative permeability to water, kₑw, and gas, kₑg [16]. In the mobile plume region, kₑw = 0 and kₑg = kₑg* < 1. In the region outside the plume, kₑw = 1 and kₑg = 0. The volumetric flux of CO₂ injected Q is assumed to be much larger than the vertically-integrated natural groundwater flow (the dimensions of Q are L²T⁻¹, reflecting that the model collapses the third dimension of the problem). The governing equation for the plume thickness during injection reads:

\[ \phi(1 - S_{wc})\partial_t h_n + \partial_x (fQ - k\Delta\rho gH\lambda_g(1 - f)\partial_x h_n) = 0, \]  

where \( \phi \) is the aquifer porosity, \( k \) is the permeability of the medium, \( g \) is the gravitational acceleration, \( f \) is the fractional flow of gas:

\[ f = \frac{h_n}{h_n + \frac{\mu_g}{k_{ew}\mu_w}(H - h_n)}, \]

where \( \mu_g, \mu_w \) are the dynamic viscosities of gas and water, respectively.

3.2. Post-injection Period

Carbon dioxide is present in the mobile plume (with saturation \( S_g = 1 - S_{wc} \)) and as a trapped phase (with residual gas saturation \( S_g = S_{gr} \)). The governing equation for the plume thickness during the post-injection period is [18]:

\[ \phi R\partial_t h_n + \partial_x (fUH - k\Delta\rho gH\lambda_g(1 - f)\partial_x h_n) = 0, \]

where \( U \) is the groundwater Darcy velocity, and \( R \) is the accumulation coefficient:

\[ R = \begin{cases} 
1 - S_{wc} & \text{if } \partial_th_n > 0 \text{ (drainage)}, \\
1 - S_{wc} - S_{gr} & \text{if } \partial_th_n < 0 \text{ (imbibition)}. 
\end{cases} \]

3.3. Dimensionless Form of the Equations

We define the dimensionless variables

\[ h = \frac{h_n}{H}, \quad \tau = \frac{t}{T}, \quad \xi = \frac{x}{L}, \]

where \( T \) is the injection time, and \( L = QT/H\phi \) is a characteristic injection distance.

During injection, the plume evolution equation is:

\[ (1 - S_{wc})\partial_\tau h + \partial_\xi (f - \frac{N_g}{Q}h(1 - f)\partial_\xi h) = 0. \]
The behavior of the system is governed by the following two dimensionless parameters:

\[
M = \frac{1/\mu_w}{k_{rg}/\mu_g} = \text{mobility ratio}, \quad N_g = \frac{k k_{rg} \Delta \rho g H}{\mu_g U (QT)/(H \phi)} = \text{gravity number}. \tag{7}
\]

Equation (6) is a nonlinear advection–diffusion equation, where the second-order term comes from buoyancy forces, not physical diffusion.

During the post-injection period, we re-scale time differently, to scale out the coefficient \( UH \) from the advection term. We choose, for \( t > T \),

\[
\tau = 1 + \frac{UH t - T}{Q}. \tag{8}
\]

The scaling in space remains unchanged. The governing equation during the post-injection period is:

\[
R \partial_{\tau} h + \partial_{\xi} (f - N_g h(1-f) \partial_{\xi} h) = 0. \tag{9}
\]

The buoyancy term reflects the difference in time scaling.

4. Analytical Solution to the Hyperbolic Model

Equations (6) and (9) can be solved using standard discretization methods. When the mobility ratio \( M \) is sufficiently small—as is the case in CO₂ sequestration scenarios—the solution is almost insensitive to the value of the gravity number [18], see Figure 3. Therefore, it is well justified to drop the second-order diffusive term from the formulation. It is interesting (but not surprising) that for \( M \ll 1 \), the solution becomes independent of the density difference between the fluids, even though it is buoyancy that sets the gravity tongue.

The case \( U = 0 \) (that is, \( N_g = \infty \)) is obviously not covered by the hyperbolic model. Numerical solutions and late-time scaling laws for this case are presented by [15]. In practice, either natural groundwater flow or aquifer slope will make the gravity number finite. The solution is then approximated by the hyperbolic model:

\[
R \partial_{\tau} h + \partial_{\xi} f = 0. \tag{10}
\]

The complete analytical solution, obtained by the method of characteristics, is shown in Figure 4. The top four figures show the profile of the plume at each stage of the CO₂ migration process: (a) injection, (b) retreat, (c) chase, and (d) sweep. The bottom figure (e) shows the solution on the dimensionless \( (\xi, \tau) \) characteristic space.

Injection Period. During injection \((0 < \tau < 1)\), and because the flux function is concave, the solution is a simple rarefaction fan that evolves in both directions (Fig. 4(c)). The solution profile at the end of injection \((\tau_1 = 1)\) is shown in Fig. 4(a), and the extent of the plume is

\[
\xi_{\text{inj}} = \frac{1}{(1 - S_{wc})M}. \tag{11}
\]

Retreat Stage. After injection stops \((\tau > 1)\), the plume migrates to the right, subject to groundwater flow. The solution for the right side of the plume (drainage front) continues to be a divergent rarefaction fan. The solution for the left side of the plume (imbibition front), however, is now a convergent fan. Each state \( h \) travels with a characteristic speed that is faster than that of drainage, because residual CO₂ is being left behind.

We define the capillary trapping coefficient

\[
\Gamma = \frac{S_{gr}}{1 - S_{wc}} \quad (\text{always } \in [0, 1]). \tag{12}
\]
At time $\tau_2 = 2 - \Gamma$, all characteristics impinge onto each other precisely at $\xi = 0$. Physically, this is the time at which the imbibition front becomes a discontinuity. The solution profile at a time $\tau < \tau_2$ is shown in Fig. 4(b).

**Chase Stage.** After the imbibition front passes through $\xi = 0$, due to the concavity of the flux function, the imbibition front is a genuine shock, that is, a traveling discontinuity. The continuous drainage front continues to propagate exactly as before. The solution during this stage is shown in Fig. 4(c). This period ends at time $\tau_3 = (2 - \Gamma)/(1 - M(1 - \Gamma))$, when the imbibition shock wave (thick red line) collides with the slowest ray of the drainage rarefaction wave (thin blue line) in Fig. 4(e). Physically, this is the time at which the CO$_2$ plume detaches from the bottom of the aquifer.

**Sweep Stage.** Once the mobile plume detaches from the bottom of the aquifer, the solution comprises the continuous interaction of a progressively faster shock with a rarefaction wave. The problem is solved if one determines the evolution of the plume thickness at the imbibition front, $h_m$, as a function of dimensionless time $\tau$. The differential equation governing the evolution of the state $h_m$ can be obtained by finding the intersection (on the $(\xi, \tau)$-space) of the imbibition shock wave corresponding to a state $h_m$ with the rarefaction ray for a state $h_m + dh_m$, and taking the limit $dh_m \rightarrow 0$. The initial condition is $h_m = 1$ at $\tau = \tau_3$. After separation of variables, the resulting integral equation is:

$$\int_{\tau_3}^{\tau} \frac{d\tau}{\tau} = \int_1^{h_m} \frac{f''(h)}{1 - f(h)/h - f'(h)} dh. \quad (13)$$

The integral in Equation (13) can be evaluated analytically, and the solution admits a closed-form expression:

$$\tau(h_m) = (2 - \Gamma)(1 - M(1 - \Gamma)) \left( \frac{M + (1 - M)h_m}{MT + (1 - M)h_m} \right)^2. \quad (14)$$

In Fig. 4(d), we plot the profile of the CO$_2$ plume at some time during the sweep stage. A representation of the solution in characteristic space is shown in Fig. 4(e). The thick red line corresponds to the imbibition front. When the imbibition front collides with the fastest ray, the entire CO$_2$ plume is in residual, immobile form. This occurs at a dimensionless time $\tau_{\text{max}} = \tau(h_m = 0)$.

**5. Footprint of the Plume**

An important practical result from the analytical solution derived above is a closed-form expression for the time scale for complete trapping,

$$\tau_{\text{max}} = \frac{(2 - \Gamma)(1 - M(1 - \Gamma))}{\Gamma^2}. \quad (15)$$

and the maximum migration distance of the CO$_2$ plume,

$$\xi_{\text{max}} = \frac{(2 - \Gamma)(1 - M(1 - \Gamma))}{\Gamma^2} \frac{1}{(1 - S_{wc}M)}. \quad (16)$$

The capillary trapping coefficient $\Gamma$ in Equation (12) emerges as the key parameter in the assessment of CO$_2$ storage in saline aquifers. It is always between zero and one, and it increases with increasing residual gas saturation. Larger values of $\Gamma$ result in more effective trapping of the CO$_2$ plume. It is not surprising that the ultimate footprint of the plume is inversely proportional to the mobility ratio $M$. The maximum migration distance is also strongly dependent on the shape of the plume at the end of the injection period, suggesting that it is essential to model the injection period for proper assessment of the ultimate footprint of the plume.
Our model also permits the determination of the storage capacity of a geologic basin, and the storage efficiency factor due to capillary trapping. Defining the efficiency factor as the ratio of the volume of CO2 injected and the pore volume of the aquifer, \( V_{\text{CO2}} = E_{\text{capil}} V_{\text{pore}} \) [19], it takes the following simple expression:

\[
E_{\text{capil}} = \frac{2}{\xi_{\text{inj}} + \xi_{\text{max}}},
\]

where \( \xi_{\text{inj}} \) and \( \xi_{\text{max}} \) are given by Equations (11) and (17), respectively.

Our analysis allows us to evaluate quickly the footprint that can be expected from a CO2 sequestration project at the basin scale. Consider an aquifer with \( k = 100 \text{ md} = 10^{-13} \text{ m}^2 \), \( \phi = 0.2 \), and \( H = 100 \text{ m} \). Injection conditions are about 100 bar and 40°C. Under these conditions, \( \rho \approx 400 \text{ kg m}^{-3} \), \( \Delta \rho \approx 600 \text{ kg m}^{-3} \), \( \mu_g \approx 0.05 \times 10^{-3} \text{ kg m}^{-1} \text{ s}^{-1} \), and \( \mu_w \approx 0.8 \times 10^{-3} \text{ kg m}^{-1} \text{ s}^{-1} \). We take the following rock–fluid property values: \( S_{\text{woc}} = 0.4 \), \( S_{\text{gr}} = 0.3 \), and \( k_{\text{rgr}}^* = 0.6 \) [20]. These parameters lead to the following values of the trapping coefficient and the mobility ratio: \( \Gamma = 0.5 \) and \( M \approx 0.1 \). Consider a major sequestration project, in which 0.2 Gigatonnes of CO2 are injected every year, for a period of \( T = 30 \) years (this scenario corresponds to the injection of the CO2 emitted by about 200 medium-size coal-fired power plants). If injection takes place at 100 wells, with interwell spacing of 1 km, then \( Q = 2500 \text{ m}^3 \text{ yr}^{-1} \), and \( Q/H = 25 \text{ m yr}^{-1} \). Assume that the background groundwater flow is \( U = 0.1 \text{ m yr}^{-1} \). The corresponding gravity number is \( N_g \approx 60 \), well within the range of validity of the hyperbolic approximation. For this set of parameters, the expected footprint of the plume and time scale for complete trapping are (in dimensionless quantities): \( \xi_{\text{strmax}} = 95 \), \( \tau_{\text{max}} = 5.7 \).

It is instructive to convert them to dimensional values: \( x_{\text{max}} = (QT/H\phi)\xi_{\text{strmax}} \approx 350 \text{ km} \), and \( t_{\text{max}} = (T+Q/UH)(\tau_{\text{max}}-1) \approx 35,000 \text{ yr} \). The corresponding value of the capillary trapping efficiency factor is \( E_{\text{capil}} \approx 1.8\% \), which, in this particular case, is in the range of 1–4% suggested by the DOE Regional Carbon Sequestration Partnerships [20,22].

6. Discussion and Conclusions

The results above suggest that it is the scale of hundreds of kilometers in space, and thousands of years in time, that is relevant for the assessment of geological CO2 sequestration at the gigatonne scale.

The applicability of the model hinges on some important assumptions and approximations. Aquifer heterogeneity, for example, will often increase the migration distance. The gravity tongue, however, is a persistent feature of the flow that is likely to dominate the picture, regardless of heterogeneity. Due to the large time scales expected, the assumption of neglecting dissolution of CO2 in the brine becomes questionable. Dissolution will decrease the migration distance and, from this point of view, the estimates of plume footprint are on the safe side. One way to accelerate the time to trap the CO2 (and make the no-dissolution and hyperbolic approximations more applicable) is to inject water slugs, along with the CO2 [5]. The model also neglects loss of CO2 through the caprock. Application of the analytical solution requires that geological features that serve as conduits for vertical fluid migration be mapped, and that the well array of Figure 1 be placed such that the plume avoids such features (which include outcrops, faults, conductive fractures, etc.)

The analytic expressions derived here have immediate applicability to obtaining flow-based capacity estimates for CO2 sequestration at the basin scale. Our analysis also provides a parsimonious, analytical and physically-based model for risk assessment under uncertainty. These applications are presented in a companion paper [22].

References


Figure 1. Schematic of the basin-scale model of CO₂ injection. The CO₂ is injected in a deep formation (blue) that has a natural groundwater flow (West to East in the diagram). The injection wells (red) are placed forming a linear pattern in the deepest section of the aquifer. Under these conditions, the North-South component of the flow is negligible, and is not accounted for in the one-dimensional flow model developed here.

Figure 2. Conceptual representation of the two different periods of CO₂ migration in a horizontal aquifer: (a) injection period; (b) post-injection period (see text for a detailed explanation).

Figure 3. Numerical solution to the full nonlinear advection–diffusion model. Shown are the profiles of the mobile CO₂ plume (white) and trapped CO₂ (light blue) at dimensionless time $\tau = 2$, for different values of the gravity number: (a) $N_g = 1$, (b) $N_g = 10$, and (c) $N_g = 100$.

Figure 4. Analytical solution to the hyperbolic model. Profiles of the mobile CO₂ plume (white) and trapped CO₂ (light blue) during the (a) injection period, (b) retreat stage, (c) chase stage, and (d) sweep stage. (e) Complete solution on $(\xi, \tau)$-space until the entire CO₂ plume has been immobilized in residual form (see text for a detailed explanation).