Dynamics of Vertical Displacement in Porous Media Associated With CO$_2$ Sequestration

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Summary
The problem of CO$_2$ sequestration in geologic formations is analyzed from a fundamental perspective. In order to clearly understand the first order behavior of the system, the mechanisms of trapping, dissolution and chemical reactions are not accounted for. The analysis is concerned with the post-injection period when the CO$_2$ plume rises due to buoyancy. Characteristics of the plume for a 1D problem show that a pair of shocks moving in opposite directions is produced at the top end. The downward moving shock interacts with the bottom end of the plume resulting in a decrease in the maximum value of the CO$_2$ saturation. High accuracy numerical simulations are employed to understand the 2D mechanisms of plume evolution in terms of the viscosity ratio and the capillary number. 2D results show that the plume rises to significantly lower depth, in shorter times, as compared to the 1D problem. This behavior is governed by the 2D velocity field around the plume that additionally leads to spanwise wave interactions and results in a faster decrease of the maximum CO$_2$ saturation. The initial dimensions of the plume have a strong influence on the time scales of the wave interactions. The maximum upward velocity that is generated due to buoyancy is closely related to the maximum saturation and decays rapidly to very small values with a decrease in saturation. In the case where the viscosity of CO$_2$ is a tenth of the viscosity of the surrounding fluid, the plume rises up about 500 m in 700 yrs. Our results provide an upper bound on the maximum rise distance and the sequestration time for the problem involving trapping and dissolution. Comparison with experimental results show that the buoyancy velocity obtained from our results is of the same order as observed in the experiments.

Introduction
The behavior of two-phase flow in porous media under conditions of unstable density stratification is an important and challenging problem applicable to many practical settings of interest. Particularly, the dynamics of two-phase immiscible flows that are gravitationally unstable play a central role in the area of carbon dioxide storage in saline aquifers and other applications. The important issue in this regard is the understanding and prediction of the fate of CO$_2$ over a time period of geological scale (Bachu et al. 1994). The success of CO$_2$ sequestration operations in subsurface geological formations is critically linked to the ability of the storage site to sequester the gas indefinitely. The main mechanisms of sequestration are microscopic residual trapping, dissolution of gas into brine, and chemical fixing of carbon into the rock (Gunter et al. 1997). Various time scales as well as the nature of the storage site determine the relative importance of these mechanisms.

The sequestration process can be broadly classified into three phases (Ennis-King and Paterson 2005). Namely, the injection phase where super-critical CO$_2$ is injected into the site. This is followed by the post-injection period where the gas rises as a buoyant plume. Residual trapping and dissolution will be of primary importance in this stage. The final stage is thought to be governed by dissolution driven gravitationally unstable flows (Riaz et al. 2006) as well as chemical reactions of CO$_2$ with the porous rock. During the initial stage, the density and viscosity of the injected gas are less than the resident brine; therefore, the flow can potentially become unstable hydrodynamically (Riaz and Tchelepi 2007) due to unfavorable contrasts of density and viscosity. The extent of the initial injection period is determined by the amount of carbon dioxide that can be stored in a given reservoir; however, this period is expected to be much shorter than the subsequent post injection period. The modeling of the injection process, which is based on the relative permeability formulation of the Darcy equations, is thought to be well developed for drainage type displacements that occur during this phase (Kumar et al. 2005). Most of the main trapping mechanisms are either unavailable or are relatively less important during the initial period. For example, residual trapping does not take place during drainage while chemical trapping occurs over much larger time scales. Viscous instability at the macroscopic scale is also a possibility (Riaz and Tchelepi 2006).

Our understanding of the evolution of the CO$_2$ plume during the post injection period is incomplete. It is during this stage that the processes of residual trapping and dissolution are expected to play a primary role. While in general one can expect the plume to rise due to buoyancy, the particular mechanisms of transport are in the initial stages of investigation (Wood et al. 2004; Stohr and Khalili 2006; Tokunaga et al. 2000). For example, what is the most appropriate model for the flow; is the relative permeability model appropriate, or given the extremely small capillary numbers, should the invasion percolation model be used (Yortsos et al. 2001)? Regardless of which model is used, the main questions that need to be addressed are: how far can the plume rise; what is the velocity of rise, and how far does the plume spread during its ascent? The last issue is important from the point of view of dissolution which occurs immediately when the gas comes into contact with unsaturated brine. However, because the saturation threshold of brine is small, a continuous supply of fresh brine around the buoyant plume can increase dissolution significantly. In this investigation we attempt to understand the dynamics of the CO$_2$ plume during the period immediately following the injection phase. We use the Darcy relative permeability model to analyze the dynamics governing the natural convection of the buoyant plume and provide some preliminary estimates of how far and how fast will the plume rise. In order to focus on the primary characteristics of transport governed by the Darcy model, we carry out the analysis for homogeneous rocks, without residual trapping and dissolution. Hence, the first order behavior of the system will be considered as a primary guide to subsequently develop a better understanding of more complex processes. A sketch of the CO$_2$ plume is shown in Fig. 1. The non-wetting gas phase is immersed in brine which is the wetting phase. A buoyancy force per unit volume $F_B$ results in upward motion with velocity proportional to $U_B$, inducing a downward flow of brine around the plume.

Equations and scaling
Two-phase immiscible flow is modeled by Darcy’s equations for each phase which can be expressed in dimensional form as,

\[
\mathbf{u}_w^* = \frac{k_{rw}}{\mu_w} (\nabla P_w^* + \rho g \hat{z}) \quad \quad \quad \quad \quad (1)
\]

\[
\mathbf{u}_n^* = \frac{k_{rn}}{\mu_n} (\nabla P_n^* + \rho g \hat{z}) \quad \quad \quad \quad \quad (2)
\]

\[
\nabla \cdot \mathbf{u}_w^* = 0 \quad \quad \quad \quad \quad (3)
\]

\[
\nabla \cdot \mathbf{u}_n^* = 0 \quad \quad \quad \quad \quad (4)
\]

\[
\nabla \cdot \mathbf{u}_w^* = -\nabla \cdot \nabla P_w^* \quad \quad \quad \quad \quad (5)
\]

\[
\nabla \cdot \mathbf{u}_n^* = -\nabla \cdot \nabla P_n^* \quad \quad \quad \quad \quad (6)
\]
In order to make the above equations dimensionless we use the plume diameter $D$ as the length scale, as shown in Fig. 1 and the buoyancy velocity $U_B$ as the velocity scale,

$$U_B = k \Delta g / \mu_w$$

Eqs. 5 and 6 in dimensionless form are

$$u^*_n = \frac{\mu_w k^*_w}{\mu_n k^*_iw + \mu_w k^*_rn} u^*_T$$

$$u^*_T = \frac{k}{\mu_w \mu_n} (\mu_w k^*_iw + \mu_w k^*_rn) \nabla P^*_n + \frac{k^*_w}{\mu_w} \left( \frac{dP^*_c}{dS_n} \nabla S_n + \Delta g \hat{z} \right)$$

where the density difference $\Delta \rho = (\rho_w - \rho_n)$. Pressure is redefined to be

$$\nabla P^*_n = \nabla P^*_n - \rho_w g \hat{z}$$

In order to make the above equations dimensionless we use the plume diameter $D$ as the length scale, as shown in Fig. 1 and the buoyancy velocity $U_B$ as the velocity scale,

$$\nabla P^*_n = \nabla P^*_n - \rho_w g \hat{z}$$

Eqs. 5 and 6 in dimensionless form are

$$u^*_n = f_n u_T - \frac{k_{iw} k_{rn}}{C_a \lambda} \frac{dP_c}{dS_n} \nabla S_n + \frac{k_{iw} k_{rn}}{\lambda} \hat{z}$$

$$u^*_T = -\lambda \nabla P + \frac{k_{iw}}{C_a} \frac{dP_c}{dS_n} \nabla S_n - k_{iw} \hat{z}$$

The endpoint values of relative permeability, $k_{iw}(0)$ and $k_{iw}(1)$, are used to scale relative permeability functions and appear in the definition of the mobility ratio $M$. The value of $M$ for the CO$_2$ sequestration problem is expected to be $\sim 10^{-1}$. The relevant scalings for the non-wetting phase pressure and the capillary pressure are,

$$P^*_n = \frac{\mu_w U_B D}{k}$$

$$P^*_c = \frac{P_c \gamma_{nw}}{\phi \lambda}$$

where $\gamma_{nw}$ is the interfacial tension, $\phi$ is the porosity and $k$ the permeability. The capillary number in the above equations is defined as

$$Ca = \frac{\mu_w U_B D}{\Delta S \sqrt{\phi} f_{nw}}$$

Equations governing the transport of the non-wetting phase and the incompressibility condition are,

$$\frac{\partial S_n}{\partial t} + \nabla \cdot u_n = 0 \hspace{1cm} (18)$$

$$\nabla \cdot u_T = 0 \hspace{1cm} (19)$$

along with the boundary conditions for an infinite domain

$$u_T = 0 \hspace{1cm} x = \pm \infty$$

$$S = s_{wi} \hspace{1cm} x = \pm \infty \hspace{1cm} (20)$$

$$\nabla P = 0 \hspace{1cm} x = \pm \infty$$

The above equations are characterized by two main nondimensional parameters which are the time, $t$, and capillary number, $Ca$. Time is scaled with $D/U_B$. These parameters can be expressed as

$$t^* = \frac{\mu_w D}{k \Delta g}$$

$$Ca = \frac{\Delta \rho g D \sqrt{\lambda}}{\Delta S \sqrt{\phi} f_{nw}}$$

Note that the capillary number is independent of viscosity and can also be expressed in terms of the Bond number as

$$Bo = \frac{\Delta \rho g d^2}{\gamma_{nw}}$$

$$Ca = \frac{Bo}{\Delta S \sqrt{d^2 k}}$$
where $d$ is some characteristic pore length $\sim O(10^{-4})$ m. Hence the capillary number in this problem can be interpreted as representing the ratio of gravity to capillary effects relative to the ratio of the microscopic to macroscopic lengths.

Some particular values of density, viscosity, and permeability relevant to the CO$_2$ sequestration problem are

\[
\Delta \rho = 10^2 \text{kg/m}^3 \\
\mu_w = 1 \times 10^{-3} \text{Pa-s} \\
\mu_n = 0.03 \times 10^{-3} \text{Pa-s} \\
\gamma_{nw} = 40 \times 10^{-3} \text{N/m} \\
\phi = 0.3 \\
\Delta S = 0.8 \\
k = 10^{-14} \text{m}^2 \\
D = 10^2 \text{m} \\
d = 10^{-4} \text{m}.
\]

Based on these values, $U_B \sim 10^{-6}$ m/s, and the dimensionless numbers are estimated to be,

\[
Bo \sim 10^{-2} \quad \text{-------------------------- (25)} \\
Ca_m \sim 10^{-6} \quad \text{-------------------------- (26)} \\
Ca \sim 10^2 \quad \text{-------------------------- (27)}
\]

Although the microscopic capillary number and the bond number are dangerously close to the regime of pore-scale instability where the use of a macroscopic Darcy model is questionable (Lenormand et al. 1988), we still use Eqs. 5 and 6 in order to obtain some estimates regarding the evolution of the plume, which can then be compared with experimental results.

**1D solution**

Before we consider the full 2D problem, it is instructive to look at 1D solutions of Eq. 18 to determine the influence of viscosity ratio and capillary number. Physically, the 1D problem can be constructed as a layer of a lighter non-wetting fluid, unbounded in the lateral extent, which is between two layers of the heavier wetting fluid. The wetting phase is not connected; hence, the plume will not rise as a whole which allows one to analyze the frontal displacements only as a function of relative permeability and the viscosity ratio. We will designate the top portion of this layer, where the heavier wetting fluid is above the lighter non-wetting fluid, as the front end, and the lower part of the layer, where the heavier fluid is below the lighter fluid, will be referred to as the back end. We assume the relative permeability and capillary functions to be

\[
k_{rn} = \left(\frac{S_n - S_{nr}}{\Delta S}\right)^2 \\
k_{rw} = \left(1 - \frac{S_n - S_{nr}}{\Delta S}\right)^2 \quad \text{-------------------------- (28)} \\
\frac{dP_c}{dS_n} = \frac{1}{k_{rn}k_{rw}} \quad \text{-------------------------- (29)}
\]

The $z$-direction component of Eq. 18 with $u_T = 0$ can be expressed as

\[
\frac{\partial S_n}{\partial t} + \frac{d}{dz} \left(\frac{1}{\lambda} k_{rw}k_{rn} - \frac{1}{Ca\lambda} \frac{\partial S_n}{\partial z}\right) = 0 \quad \text{-------------------------- (31)}
\]

Eq. 31 is a weakly parabolic equation for large $Ca$. Similar to the purely hyperbolic case, $Ca \rightarrow \infty$, the solution develops along characteristics based on the flux function $f_s = k_{rw} k_{rn} / \lambda$. The flux function is plotted as a function of the non-wetting saturation in Fig. 2 for various values of the mobility ratio. The curves show that $f_s$ has a maximum value, which indicates a zero wave speed at that saturation. This leads to the development of two shocks with opposite speeds at the front end. The upward moving shock spans saturations $0 < S_n < s_u$, while the downward moving shock develops for $s_d < S_n < S_{nr}$, where $s_u$ and $s_d$ are the shock saturations for the upward and downward moving shocks, respectively. A rarefaction wave develops for $s_u < S_n < s_d$. The interface motion at the back end is characterized by a single shock spanning all saturations. The flux function for the $M = 1/10$ case, that is when the plume is less viscous than brine, shows the shock speeds are highest compared to the $M = 1$ and $M = 10$ cases. Speeds of the upward and downward moving shocks are equal when $M = 1$, while the former moves...
faster (slower) at $M = 10$ ($M = 1/10$).

The solution to this Riemann problem can be easily obtained through either the method of characteristics, or by employing appropriate flux splitting in a numerical solution, as long as the downward moving shock does not interact with the back end. Complex wave patterns are generated subsequent to this event such that obtaining the solution either by the method of characteristics or through the explicit flux correction, is not only tedious, but the correct entropy solution may also not be obvious. Because we have capillary dispersion, we include it to obtain the correct entropy solution for all wave interactions, both in the 1D and 2D problems.

The solution to Eq. 31 is plotted in Fig. 3 for various values of $M$. The initial condition is a pulse of unit length positioned at $z = 0$ with $S_{n1} = 0.8$ and $S_{n0} = 0$. In the case of $M = 1$, the shock speeds are equal; the upward and downward moving shocks bifurcate symmetrically about the stationary point. The saturation profile for the stable $M = 10$ case is relatively less developed due to small shock speeds, as indicated in Fig. 2. For the unstable viscosity case, $M = 1/10$, which has the highest shock speeds, the saturation profile indicates that the downward moving rear shock has already reached the back end. Because at the back end, the rear shock cannot go any further so that the saturation begins to decrease to preserve the correct entropy solution, subsequently leading to an increase in the front speed which conserves mass.

When the maximum saturation at the back end has decreased below the saturation associated with $dF_{nw}/ds_n = 0$, the back end is free to move in the upward direction according to $f_{nw}$. This behavior is shown in Fig. 3 for the $M = 1/10$ case. Reduction in the maximum saturation also occurs at later times for the $M = 1$ and $M = 10$ cases.

The simulation is stopped when the maximum saturation reaches a threshold value of $S_2 = 0.2$. Although the saturation can be made to approach zero, we stop the simulation at some small value to represent the finite rise of the plume in the presence of trapping. Hence, the time required to reach the threshold saturation and the distance the plume has moved during that time, provide an upper bound for the case with trapping. Saturation profiles at the final time, $t_f$, when the maximum saturation is at the threshold values, $s_2$, are shown in Fig. 4 for various values of $M$. The values of $t_f$ corresponding to $M = 1$, 10 and 1/10, are 31.5, 46.5, and 12.5, respectively. Although the fronts have traveled more or less the same distance during this time, the actual time required is more for the viscously stable $M = 10$ case. The saturation profile for the $M = 10$ case shows that the forward and rear shocks are still separated by saturations that do not belong to either shock. On the other hand, for the $M = 1$ case, the faster moving rear end has almost eliminated all saturations outside the shock at the forward end, while only the forward shock exists for the $M = 1/10$ case.

The decay of the maximum saturation $s_{max}$ occurs due to the interaction of the downward moving shock with the back end of the plume. The time evolution of $s_{max}$ provides insight into how that
interaction proceeds. Fig. 5 shows the decay of the maximum saturation with time for various values of $M$. We have also plotted corresponding values at a different capillary number to understand the effect of $Ca$ on the decay of $s_{\text{max}}$. For the $M = 1/10$ case the decay is rapid and $s_{\text{max}}$ reaches $s_f$ in a short time. During its descent, the maximum saturation goes through two periods of rapid decay, in between intervals of relatively mild decrease. This pattern is also observed at other values of $M$, (see Fig. 5), but at later times. In fact, for the $M = 10$ case only the first phase of rapid decay is observed. This interesting behavior results from the fact that the first period of fast decrease in $s_{\text{max}}$ occurs when the rear shock moves backward and reduces the saturation to a level where the back end becomes mobile. Thereafter, the back end moves upward at a higher speed than the forward shock resulting in another wave interaction, again leading to an enhanced decay of $s_{\text{max}}$. Small capillary numbers mask periods of sharp decay resulting in an almost uniformly decreasing trend for all time, at least for the $M = 1/10$ case. Moreover, in this case the time required to reach $s_f$ is the same for $Ca = 125$ and $Ca = 1000$ cases. Interestingly, had a higher threshold value been selected, a smaller capillary number would have led to a smaller value of $s_f$. For the $M = 1/10$ case, the capillary number is in fact, for the $M = 10$ case deviates from the steep decrease in $s_{\text{max}}$ and results in a smaller values of $s_f$. Therefore, this behavior indicates that depending on the threshold saturation, and by analogy the residual non-wetting phase saturation, the final time for the sequestration of a given amount of CO$_2$ can be affected significantly by the capillary number, at least in this 1D model.

The propagation of the forward shock is of interest for the sequestration problem. The maximum position that the saturation reaches ($s_f$) at the final time ($t_f$) determines how large a storage site needs to be for a given amount of CO$_2$. The characterization of the front position as a function of various parameters is hence of considerable importance. Fig. 6 shows the position of the front, $s_f$, defined to be the location of the saturation $0.1s_{\text{max}}$, for different values of $M$ and $Ca$. The front for the $M = 1$ case moves the farthest, while for $M = 1/10$ and $M = 10$ cases it progressively lags behind. Because the slope of $s_f$ vs. $t$ is the velocity of the front, Fig. 6 shows that the velocity is highest in the case of $M = 1/10$. Interestingly, even though the front velocity is larger, the front does not travel as far as in the $M = 1$ case. The slope of $s_f$ for both the $M = 1$ and $M = 10$ cases is constant, while that for the $M = 1/10$ case shows a reduction following the interaction of the back end with the forward shock. Finally, Fig. 6 shows that the influence of the capillary number is quite small.

2D dynamics

We now present numerical simulations of 2D plumes as shown in Fig. 1. Unlike the 1D case presented in the previous section, the plume will have a positive upward velocity due to the buoyancy force. Capillary and permeability drag forces act in the opposite direction, and the rise velocity of the plume will be set by the balance of these forces. We solve Eqs. 18 and 19 with boundary conditions Eq. 20. The total velocity equation is expressed in terms of the vorticity variable to avoid having to deal with pressure and to be able to resolve velocity components from Eqs. 34 and 35. The gradients in the $z$ and $x$-directions are evaluated using 8th order compact finite difference discretization using anti-symmetric boundary conditions. The domain extents $A_x = 10$ and $A_z = 5$ were found to provide a sufficient approximation to an infinite space.

The transport Eq. 18 is solved with a 4th order Runge-Kutta method. The spatial derivatives are evaluated with an 8th order accurate compact finite difference discretization. The simulation is started with a circular plume of unit diameter centered at $(z = 0, x = 0)$. The initial plume is slightly diffused to avoid discontinuities in saturation. Initial velocities are prescribed as $w = 0, u = 0$ at $t = 0$. We use sufficient grid points to accurately resolve the steep gradients at the fronts.

Fig. 7(a) shows the contour plots of saturation at an early time of $t = 1$ for $M = 1$ and $Ca = 250$. The plume has progressed slightly from its initial position leaving behind a wake of small saturation values. The location of the higher saturation values has shifted towards the back end, similar to the 1D case discussed in the previous section. Due to the generation of spanwise velocity in the 2D case, the plume profile appears to bulge slightly in the $x$-coordinate. Fig. 7(b) shows the plume profile at a later time $t = 6$. The plume has traveled upward about 5 nondimensional units at this time. The shape of the plume has deviated significantly from the circular initial profile to attain a pointed tip followed by a broader tail. Velocity vectors plotted in Fig. 7 show that at an early time the magnitude of the spanwise velocity is comparable to the streamwise component which generates a significant recirculation around the plume. At a later time, Fig. 7(b) shows that the streamwise component is dominant and the spanwise velocity is concentrated only at the tip of the plume. Hence, the ability of the plume to induce downward motion in brine is significantly reduced at later times. As for the 1D case, the simulation is stopped when the threshold saturation $s_f = 0.2$ is reached.

The saturation contours of the plume for $M = 10$ and $M = 1/10$ are shown in Fig. 8(a) and (b), respectively, with $Ca = 250$, at times close to $t_f$. The plume has traveled slightly farther for the $M = 10$ case. The $M = 1/10$ case shows a broadening of the rear section and a narrowing of the tip. However, the $M = 10$ case shows that the plume tends to retain its initial shape with a slight bulging along the spanwise direction. The region of small saturations trails both
Fig. 7—Non-wetting phase saturation contour at an early time (top), and at threshold saturation (bottom), for the 2D case at $M = 1$ and $Ca = 250$. Arrows represent the velocity field induced around the naturally buoyant plume.

Fig. 8—Non-wetting phase saturation contour for $M = 10$ (top) and $M = 1/10$ (bottom). Arrows represent the velocity field induced around the naturally buoyant plume.
plumes, but is more prominent for the $M = 10$ case. The velocity vectors show a behavior similar to the $M = 1$ case. High upward velocities are produced in regions of high saturation, and the spanwise velocities are localized around the tip of the plume. However, since the plume has stretched out considerably less in the $M = 10$ case, as compared to the $M = 1/10$ case, the induced motion of the brine is fairly uniform around the plume.

Motion of the 2D plume is obviously influenced by the buoyancy velocity generated due to the density contrast. Hence, one would expect, compared to the 1D case, that the plume will tend to propagate much higher into the brine phase. The progress of the tip position $z_f$ is plotted in Fig. 9. The results obtained for the 1D case are also shown. Surprisingly, Fig. 9 shows that the plume actually ascends less in 2D than in 1D. Although $z_f$ increases much more rapidly in the 2D case, indicating a higher upward velocity due to buoyancy, the threshold saturation is reached at an earlier time for all $M$ values, compared to the 1D case. Hence, the plume can only travel about half as much compared to its 1D counterpart. 2D results indicate that the slope of $z_f$ remains approximately constant throughout the simulation for the $M = 10$ case. On the other hand, the slope begins to decrease slightly for $M = 1$ and considerably more for $M = 1/10$. This indicates that the buoyancy generated upward velocity decreases with time such that for $M = 1/10$ the slope of $z_f$ tends to drop to the 1D level, indicating that subsequent upward motion is due only to wave propagation based on the flux function, rather than a result of buoyancy induced motion.

Accelerated decay of the maximum saturation is the cause of significantly smaller values of $t_f$ in the 2D case. The evolution of $s_{\text{max}}$ in time, as plotted in Fig. 10 shows that to be the case. The maximum saturation values for all $M$ cases decay at a considerably higher rate compared to the 1D results. This leads to small $t_f$ values and limits the plume migration to smaller distances from the origin. There are two main reasons for this behavior. The first is related to mass balance, because the asymmetric upward velocity field in the plume as well as the spanwise velocity lead to a stretching of the plume, and that causes $s_{\text{max}}$ to drop faster than in the 1D case. Secondly, the circulation generated around the plume results in spanwise velocity directed inward, towards the plume, from the brine. This leads to the motion of lateral saturation waves toward each other, where, upon subsequent interaction, the maximum saturation decays quickly. Therefore, in addition to the wave interaction in the streamwise direction, the 2D dynamics are influenced by the spanwise motion and interaction of saturation waves, resulting in a significant reduction in the final time $t_f$ compared to the 1D case.

An important characteristic regarding the plume motion is the magnitude of the upward velocity generated due to buoyancy. If this velocity is constant, then the plume can rise indefinitely in the absence of residual trapping, as long as a sufficient level of density difference between the fluids is present. In order to determine how does the upward velocity behave during the rise of the plume and how far can the buoyancy force lift the plume, we plot the maximum values of velocity for both the $w$ and $u$-components in Fig. 11. The maximum streamwise velocity has the highest magnitude for the $M = 1/10$ case, followed by $M = 1$ and $M = 10$ cases. Only in the case of $M = 1$ is this velocity related entirely to the density contrast. However, even in this case the non-monotonicity of the mobility, $\lambda$, profile (Riaz and Tchepeli 2004) contributes to vorticity generation and adds to the buoyancy driven velocity. The $M = 10$ case has the smallest velocity at the onset due to the favorable viscosity difference at the top of the plume, which subtracts from the buoyancy generated velocity.

The maximum magnitude of both the streamwise $w$ and the spanwise $u$-component decays, throughout the simulation for $M = 1$ and $M = 1/10$ cases, and at later times for the $M = 10$ case. This trend appears to correlate somewhat with the decrease in the maximum saturation as shown in Fig. 10. In fact, an almost constant velocity for the $M = 10$ case during the early times is clearly related to the time interval when the forward and the rear shocks are separated. The spanwise components have a slightly smaller magnitude than the streamwise counterparts but they follow a similar trend throughout the simulation. Hence, we see that the buoyancy induced velocity, in conjunction with the contribution from the viscosity contrast, is not constant during the motion of the plume. Rather, a uniform decrease in both components results in significantly smaller velocities at later times. A comparison with Fig. 10 shows that the rate of decrease in the maximum values of $w$ and $u$, corresponds to the period of decrease in the maximum saturation. The rate of decrease during the initial period for the $M = 1$ and $M = 1/10$ cases is proportional to $t^{-1/2}$, as shown by the slope of the dotted line in Fig. 11.
we see that the critical density difference required to overcome capillary resistance is

$$\Delta \rho_c = \frac{8 d \gamma_{nw}}{g D^2}$$ \hspace{1cm} (40)$$

where, $d$ is the average pore diameter and $D$ is the plume diameter. We have assumed a unit length in the third dimension. The value of $d$ is only an estimate of the average pore dimensions, which can be much larger or smaller at particular locations. The critical density difference required for initiating upward motion is quite small $\sim 10^{-5}$. Conversely, the critical diameter of the plume, with $\Delta \rho = 10^2 \text{kg/m}^3$ is on the order of a few millimeter.

| Table 1—Dimensional values of the time $t^*_f$ required to reach the maximum height $z^*_f$, for various values of $M$ and Ca. Results for both 1D and 2D problems are noted. |
|--------------|--------|-----------------|-----------------|-----------------|
| $M$          | Ca     | 1D              | 2D              |
|              |        | $t^*_f$ (yrs) $\times 10^3$ | $z^*_f$ (m) $\times 10^3$ | $t^*_f$ (yrs) $\times 10^3$ | $z^*_f$ (m) $\times 10^3$ |
| 1            | 125    | 1.84 $\times 10^3$ | 8.78 $\times 10^3$ | 0.64 $\times 10^3$ | 4.20 $\times 10^3$ |
| 250          | 2.40 $\times 10^3$ | 9.42 $\times 10^3$ | 0.80 $\times 10^3$ | 5.26 $\times 10^3$ |
| 500          | 2.12 $\times 10^3$ | 9.70 $\times 10^3$ | 0.92 $\times 10^3$ | 6.03 $\times 10^3$ |
| 10           | 125    | 4.00 $\times 10^3$ | 8.27 $\times 10^3$ | 1.26 $\times 10^3$ | 4.20 $\times 10^3$ |
| 250          | 3.87 $\times 10^3$ | 8.11 $\times 10^3$ | 1.76 $\times 10^3$ | 5.53 $\times 10^3$ |
| 500          | 3.63 $\times 10^3$ | 7.83 $\times 10^3$ | 2.04 $\times 10^3$ | 6.10 $\times 10^3$ |
| 1/10         | 125    | 1.00 $\times 10^3$ | 6.91 $\times 10^3$ | 0.48 $\times 10^3$ | 3.82 $\times 10^3$ |
| 250          | 0.66 $\times 10^3$ | 7.18 $\times 10^3$ | 0.61 $\times 10^3$ | 4.70 $\times 10^3$ |
| 500          | 1.03 $\times 10^3$ | 6.94 $\times 10^3$ | 0.70 $\times 10^3$ | 5.09 $\times 10^3$ |

The rise velocity of gas bubbles has been estimated by Corapcioglu et al. (2000) based on observations in artificial porous media with a constant pore size dimension (Roosevelt and Corapcioglu 1998). The phenomenon of wave interaction and the consequent decrease in the maximum saturation and reduction in rise velocity were not observed. The mathematical model used by these authors does not incorporate relative permeability but employs a balance between the buoyancy, capillary, and drag forces to compute the steady state and transient rise velocities. According to their estimate the terminal rise velocity, $U_B$, expressed in terms of our analysis is

$$U_B = \left( \frac{\Delta \rho - \frac{3R \gamma_{nw}}{2D^2}}{150 \mu_{nw} (1-\phi)^2} \right) \frac{d^2 \phi^3}{(1-\phi)^2}$$ \hspace{1cm} (41)$$

where $R = (2\sqrt{3}-3) d / 6$, and a value of $d = 4 \text{mm}$ was used. Based on Eq. 41 the rise velocity $U_B \sim 2.74 \text{ m/s}$ is obtained. On the other hand, in our case the rise velocity is $\sim 10^{-6} \text{m/s}$. This is because the permeability value in Eq. 41 is quite large, $k = 8.39 \times 10^{-9}$. Using this permeability value and the non-wetting phase viscosity to scale the rise velocity in Eq. 8, an exact match is obtained since our dimensionless velocity is order 1 for the $M = 1/10$ case at early time.

**Conclusions**

We performed a basic analysis of the CO$_2$ plume problem that highlights the first order behavior of the system. The 1D solution of the problem indicates that the plume bifurcates into an upward moving and a downward moving shock, based on the type of the flux function used. The downward moving shock interacts with the bottom end of the plume, reducing the maximum saturation as a result. This type of wave interference is strictly governed by the flux function and is therefore entirely dependent upon the functional form of relative permeability functions.

The analysis of the 2D problem shows that the wave interference occurs both in the case of streamwise moving as well as spanwise moving shocks. This results in a more rapid decrease of the maximum saturation as compared to the 1D case. Interestingly, the upward moving forward end of the plume rises to about half the level
of the corresponding 1D case due to the enhanced reduction in the maximum saturation.

Capillary dispersion plays a small role in determining the final time and the maximum height reached by the plume. Larger values of \( Ca \), indicating less capillary dispersion, result in slightly larger values of the final time and the maximum migration distance. Moreover, the trend is toward less influence of capillary dispersion for larger values of \( Ca \).

Because we neglected capillary trapping, we had to stop the simulation when the maximum saturation was reduced to some specific value. If one interprets this threshold saturation as the residual or trapped saturation, then our results can be used as a prediction for the upper bounds in the final time and the maximum height. The effect of trapping will be to further reduce these values than can be achieved without trapping. Another mechanism of importance is the dissolution of \( CO_2 \) in brine which has the effect of increasing the density of saturated brine while keeping the volume approximately the same. The heavier saturated brine will sink generating a stronger circulation current around the plume. The strengthened circulation will have the added effect of inducing more fresh brine around the plume, which would further increase the circulation in a nonlinear feed back loop. 3D effects are another potential avenue in which to extend the current analysis. However, introduction of the third dimension might not affect the results as dramatically as in which to extend the current analysis. However, introduction of the third dimension might not affect the results as dramatically as moving from 1D to 2D. Finally, the applicability of the Darcy representation of drainage needs to be clearly established, because the Bond numbers and the capillary numbers for the \( CO_2 \) sequestration problem are very similar to the cases where microscopic instability is observed.

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References


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