# MOMENT EQUATIONS FOR STOCHASTIC IMMISCIBLE FLOW

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**Abstract.** We derive and analytically and numerically solve statistical moment differential equations for immiscible flow in porous media in the limit of zero capillary pressure, with application to secondary oil recovery. Closure is achieved by Taylor expansion of the fractional flow function and a perturbation argument. We reduce the equations by exploiting a relationship between saturation and velocity correlations that is unique to flow in one dimension. Mean and variance of (water) saturation exhibit a bimodal character; two shocks replace the single shock front evident in the classical Buckley–Leverett saturation profile. [1]

**Key words.** porous media, stochastic, random fields, moment equations

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## 1. Introduction.

Subsurface geologic properties at field scales are uncertain, and are often described statistically in practice. Flow profiles in such porous media are uncertain, and statistical flow outcomes are appropriate. We are primarily interested in mean behavior and a measure of the uncertainty about this mean.

A "zeroth-order" model of mean flow with averages of geologic properties ignores correlations between flow variables. Monte Carlo simulations of many realizations of geologic properties to estimate moments require much computation time and careful sampling techniques [12, 13, 35]. Macrodispersion theory in contaminant transport captures a first-order effect of fluctuations via covariance functions in PDEs for the mean concentration [7, 14]. This theory has a long history in subsurface contaminant transport, and is closely related to eddy diffusion models of turbulence [16, p. 358 ff].

We derive second-order PDEs for the covariance functions and the mean flow, and solve for these moments simultaneously. The fundamental problem of closure of the system is addressed by a perturbation argument. The resulting *moment differential equations* (MDEs) directly approximate the local mean and covariance functions, for general boundary conditions and general stochastic geology [38].

### 1.1. Applications.

A statistical description of subsurface flow is of particular interest for secondary oil recovery. The principal difficulty is a non-convex nonlinear flux function in an advection equation that leads to discontinuous solutions. Standard pressure–saturation equations for 2-D horizontal flow of two immiscible fluids in porous media, in the limit of vanishing capillary pressure ($p_c = 0$), are

$$\phi\,\mathbf{v}(\mathbf{x}) = -\mathbf{K}(\mathbf{x})\,\nabla h(\mathbf{x}), \qquad \nabla\cdot\mathbf{v}(\mathbf{x}) = 0, \tag{1.1}$$

$$\partial_t s(\mathbf{x},t) + \nabla\cdot[f(s(\mathbf{x},t))\mathbf{v}(\mathbf{x})] = 0. \tag{1.2}$$

These are taken to be valid from *laboratory* (centimeters) to *field* scales of reservoir depth (10-100 meters) and length (100-1000 meters). Hydraulic conductivity $\mathbf{K}$ may

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be an anisotropic tensor; here, for simplicity, it will be an isotropic scalar $K$. Assume also that $K$ depends weakly on (water) saturation $s$ [1, 3]. Apply (1.1)–(1.2) to the flow of oil and water, for arbitrary fluid mobilities. Denote the *total velocity*, a scaled total volumetric flux of both fluids, by $\mathbf{v}$, hydraulic water head by $h$, and porosity (assumed constant) by $\phi$. The *fractional flow function* $f(s)$, for $p_c = 0$, represents the fraction of $\mathbf{v}$ due to water. It is typically S-shaped, and we use a form arising from quadratic relative permeabilities for illustration (see [1]). However, our method does not depend on any such specific choice of $f(s)$.

Capillary pressure regularizes sharp fronts caused by the nonlinear advection term. To obtain a linear approximation to this effect, add $\epsilon_D \nabla^2 s(\mathbf{x}, t)$ with $\epsilon_D > 0$ to the right side of (1.2). Letting $\epsilon_D \to 0$ defines the *vanishing-viscosity* solution [33], which is the one we seek.

As is standard in subsurface applications, let $Y = \ln K$ be a random field with prescribed mean and covariance functions; e.g., it is often claimed that $Y$ is multivariate Gaussian, based on empirical observations [10] (our method does not depend on this). Through (1.1)–(1.2), $\mathbf{v}$ and $s$ are thus random fields. No other underlying sources of uncertainty are considered in this study.

Under the assumptions stated above, with steady boundary conditions, and neglecting the weak dependence of $K$ on $s$, a steady $\mathbf{v}$ can be determined from (1.1). We evolve $s$ from the stochastic PDE (1.2), assuming known statistics of $\mathbf{v}$. Moments of $\mathbf{v}$ and $h$ can be estimated from established theory ([36–38, 41] use MDEs). We combine analytical and numerical techniques to model the propagation of uncertainty from an underlying random field $Y(\mathbf{x})$, through $\mathbf{v}(\mathbf{x})$, to the solution $s(\mathbf{x}, t)$.

**1.2. Previous work.** Existing work on MDEs focuses mostly on advection equations with linear flux functions [15], and some nonlinear subsurface flow equations of a form different from (1.2) [2, 34, 36, 37, 41].

Langlo and Espedal [22, 23] presented a macrodispersion approach for the stochastic version of (1.2). The flux function is expanded in a Taylor series, and high-order terms are neglected; then standard techniques represent macrodispersivity as a function of flow velocity covariance. Zhang, Tchelepi, and Li take advantage of the steady velocity field, and transform 2-D flow to 1-D Lagrangian flow along streamlines [39, 40]. They formulate integral equations for moments from ensemble averages over the streamlines, rather than a system of MDEs. Variations on the streamline approach are currently popular in subsurface transport [6, 8, 9, 31, 32].

An Eulerian MDE approach has been successful for single- and multiphase pressure and velocity equations [36], and a natural next step is to extend the theory from flux equations to transport equations. This framework differs from streamlines not only in formulation, but also in that the MDEs need no velocity-distribution assumption, and an extension to transient velocity fields is relatively straightforward. The approach applies to any probability distribution of geologic properties and any correlation function, and does not require stationarity. Other stochastic theories generally require such restrictions.

Equations are derived in §2. In §3, we reduce the mean and variance equations to a simple form. These are shown to be strictly hyperbolic for 1-D flow, and an analytical solution is given in §4. The uniqueness of solutions to hyperbolic PDEs is considered. Classification is briefly discussed for 2-D equations. We conclude with an evaluation of our results and their practical implications, and a brief overview of additional questions that warrant future investigation.

**2. Moment Equations.** We compare two different approaches for statistical MDEs of 1-D flow. In §2.1, we expand fields in the form $u = \langle u \rangle + \delta u$ and the resulting MDEs are closed by neglecting products of '$\delta$' terms. Analogous equations in §2.3 result from a full asymptotic expansion. We show in §4 that the latter yields moments that violate physical constraints. In both cases, random fluctuations in $Y = \ln K$ are assumed small: $\sigma_Y \ll 1$. We can immediately generalize to higher dimensions via vector notation. Moments of $h$ and $\mathbf{v}$ are assumed known from (1.1) and moments of $Y$.

The 1-D saturation equation (1.2), with initial data $s(x,0) = g(x)$, is

$$\partial_t s + \partial_x (f(s)v) = 0, \tag{2.1}$$

We assume that $g$ is known with certainty. Solutions are defined in terms of vanishing viscosity as in §1.1; henceforth, this is tacitly understood. Incidentally, (2.1) can be solved exactly, and moments computed by integrating against a known probability density. This is carried out in [39] and [40], for example. However, since we ultimately develop Eulerian equations for moments in two and three space dimensions with spatial dependence in the velocity, we apply the approach to the 1-D equation first.

**2.1. Two-term expansion.** Moment equations may be derived in a number of ways. For examples of commonly used methods applied to various models in subsurface flow and transport, see [7, 11, 14, 15, 30, 36]. These methods originated in the correlation equations of turbulence models. Here we apply a standard approach, separating mean fields from random fluctuations.

Let $\langle \cdot \rangle$ denote the expectation operator, defined by

$$\langle \psi \rangle \equiv \int_\Omega \psi(\omega)\, dP(\omega) \tag{2.2}$$

for any integrable function $\psi : \Omega \to \mathbb{R}$ on the sample space $\Omega$ with probability measure $P$. We omit reference to $\omega$ in what follows.

The random field $Y$ is decomposed into deterministic mean plus random fluctuation: $Y = \langle Y \rangle + \delta Y$. Each field dependent on $Y$ is represented similarly:

$$\begin{gathered} h(x) = \langle h \rangle (x) + \delta h(x), \qquad v(x) = \langle v \rangle (x) + \delta v(x), \\ s(x,t) = \langle s \rangle (x,t) + \delta s(x,t). \end{gathered} \tag{2.3}$$

Recall that we only need the decompositions of $v$ and $s$ here. Next, the fractional flow function is expanded in a Taylor series around $\langle s \rangle$:

$$f(s) = f(\langle s \rangle) + f'(\langle s \rangle)\delta s + \frac{1}{2} f''(\langle s \rangle)\delta s^2 + \cdots \tag{2.4}$$

So far, we make no assumption regarding the size of $\delta s$ relative to $\langle s \rangle$.

To obtain the mean-saturation equation, apply the operator $\langle \cdot \rangle$ to (2.1):

$$\begin{aligned} \partial_t \langle s \rangle + \partial_x \Big[ & f(\langle s \rangle) \langle v \rangle + f'(\langle s \rangle) \langle \delta s\, \delta v \rangle + \frac{1}{2} f''(\langle s \rangle) \langle v \rangle \langle \delta s^2 \rangle \\ & + \frac{1}{2} f''(\langle s \rangle) \langle \delta s^2 \delta v \rangle + \frac{1}{3!} f'''(\langle s \rangle) \langle v \rangle \langle \delta s^3 \rangle + \cdots \Big] = 0. \end{aligned} \tag{2.5}$$

The flux terms include a nonlinear advective mean, two covariances, and higher-order moments. For the saturation-fluctuation equation, subtract (2.5) from (2.1):

$$\partial_t \delta s + \partial_x \Big[ f(\langle s \rangle)\delta v + f'(\langle s \rangle)\delta s \langle v \rangle + f'(\langle s \rangle) \left(\delta s\, \delta v - \langle \delta s\, \delta v \rangle\right) \\ + \frac{1}{2} f''(\langle s \rangle) \langle v \rangle \left(\delta s^2 - \left\langle \delta s^2 \right\rangle\right) + \frac{1}{2} f''(\langle s \rangle) \left(\delta s^2 \delta v - \left\langle \delta s^2 \delta v \right\rangle\right) + \cdots \Big] = 0. \quad (2.6)$$

We derive equations for the unknown covariance functions $\langle \delta s \delta v \rangle$ and $\left\langle \delta s^2 \right\rangle$, using the following additional notation. The independent variables are $x$ and $t$ except where noted, and $\cdot|_y$ denotes the replacement of $x$ by some $y$ different from $x$. It is convenient and useful to derive equations for the more general two-point covariances $\langle \delta s \delta v|_y \rangle$ and $\langle \delta s \delta s|_y \rangle$ rather than for one-point covariances.

To obtain an equation for the saturation-velocity covariance $\langle \delta s \delta v|_y \rangle$, multiply (2.6) by $\delta v(y)$ and apply $\langle \cdot \rangle$. This results in:

$$\partial_t \langle \delta s \delta v|_y \rangle + \partial_x \Big[ f(\langle s \rangle) \langle \delta v\, \delta v|_y \rangle + f'(\langle s \rangle) \langle v \rangle \langle \delta s\, \delta v|_y \rangle + f'(\langle s \rangle) \langle \delta s \delta v\, \delta v|_y \rangle \\ + \frac{1}{2} f''(\langle s \rangle) \langle v \rangle \left\langle \delta s^2 \delta v|_y \right\rangle + \frac{1}{2} f''(\langle s \rangle) \left\langle \delta s^2 \delta v\, \delta v|_y \right\rangle + \cdots \Big] = 0. \quad (2.7)$$

Similarly, multiplying (2.6) by $\delta s(y,t)$, and using the identity[2] $\partial_t (\delta s \delta s|_y) = \delta s \partial_t \delta s|_y + \delta s|_y \partial_t \delta s$, yields this equation for the two-point saturation covariance:

$$\partial_t \langle \delta s \delta s|_y \rangle + \partial_x \Big[ f(\langle s \rangle) \langle \delta s|_y \delta v \rangle + f'(\langle s \rangle) \langle v \rangle \langle \delta s\, \delta s|_y \rangle + f'(\langle s \rangle) \langle \delta s\, \delta v\, \delta s|_y \rangle \\ + \frac{1}{2} f''(\langle s \rangle) \langle v \rangle \left\langle \delta s^2 \delta s|_y \right\rangle + \frac{1}{2} f''(\langle s \rangle) \left\langle \delta s^2 \delta v\, \delta s|_y \right\rangle + \cdots \Big] \quad (2.8) \\ + \partial_y \Big[ f(\langle s|_y \rangle) \langle \delta s\, \delta v|_y \rangle + f'(\langle s|_y \rangle) \langle v|_y \rangle \langle \delta s|_y \delta s \rangle + f'(\langle s|_y \rangle) \langle (\delta s\, \delta v)|_y \delta s \rangle \\ + \frac{1}{2} f''(\langle s|_y \rangle) \langle v|_y \rangle \left\langle \delta s^2|_y \delta s \right\rangle + \frac{1}{2} f''(\langle s|_y \rangle) \left\langle (\delta s^2 \delta v)|_y \delta s \right\rangle + \cdots \Big] = 0.$$

**2.2. Closure by perturbation argument.** If $\sigma_Y \ll 1$ so that fluctuations and their derivatives may be assumed small relative to the means, and if $f$ is smooth, then we can approximate (2.5)–(2.8) by a closed, coupled system. Defining $c_{sv}(x,y,t) = \langle \delta s \delta v|_y \rangle$, $c_s = \langle \delta s \delta s|_y \rangle$, $c_v = \langle \delta v \delta v|_y \rangle$, $\langle s \rangle |_y = \langle s \rangle (y,t)$, and $\widehat{c}_{sv}(x,y,t) = c_{sv}(y,x,t)$, the resulting system is

$$\partial_t \langle s \rangle + \partial_x \Big[ f(\langle s \rangle) \langle v \rangle + f'(\langle s \rangle)\sigma_{sv} + \frac{1}{2} f''(\langle s \rangle)\sigma_s^2 \langle v \rangle \Big] = 0, \quad (2.9a)$$

$$\partial_t c_{sv} + \partial_x \Big[ f(\langle s \rangle) c_v + f'(\langle s \rangle) \langle v \rangle c_{sv} \Big] = 0, \quad (2.9b)$$

$$\partial_t c_s + \partial_x \Big[ f(\langle s \rangle) \widehat{c}_{sv} + f'(\langle s \rangle) \langle v \rangle c_s \Big] + \partial_y \Big[ f(\langle s \rangle|_y) c_{sv} + f'(\langle s \rangle|_y) \langle v|_y \rangle c_s \Big] = 0. \quad (2.9c)$$

Initial data are $\langle s \rangle (x,0) = g(x)$, $c_{sv}(x,y,0) = c_s(x,y,0) = 0$; recall that $\langle v \rangle$ and $\langle \delta v \delta v|_y \rangle$ are assumed known. Both (2.9b) and (2.9c) have advective flux terms, are coupled to the mean equation (2.9a), and are first-order in $\sigma_Y^2$. This is consistent with the approximation to (2.9a), which is second-order in $\sigma_Y$.

[2]The identity is not valid in a strong sense for discontinuous solutions. Recall, however, that we define solutions in terms of the (smooth) viscous solution, in the limit $\epsilon_D \to 0$.

Another common closure argument, which may be called a Gaussian assumption, might be applied here. For example, for the linear case ($f(s) = s$), (2.9) is exact if one assumes that velocity and saturation are jointly multivariate normal [11]. This follows without a perturbation argument. The linear case under this assumption is studied in [15], with the inclusion of small-scale diffusion. Using simulations, we found that the Gaussian assumption, even for transformations of saturation and velocity fields, is inappropriate for this problem [18]. That result also prohibits the convenience of modeling a transformation of $f(s)$ as Gaussian rather than using a Taylor expansion (a similar approach was used successfully for unsaturated flow in [2]).

Note that the mean equation (2.9a) contains the functions $\sigma_{sv} = c_{sv}(x,x,t)$ and $\sigma_s^2 = c_s(x,x,t)$ rather than $c_{sv}(x,y,t)$ and $c_s(x,y,t)$. This mix of one-point and two-point covariance functions prevents us from immediately treating the MDEs as classically hyperbolic, even though they can be put in conservation-law form. Also, independent variables $x$ and $y$ are permuted in $\langle s \rangle$ and $c_{sv}$ in (2.9c). In general, $\langle s \rangle |_y \neq \langle s \rangle$, and $\widehat{c}_{sv} \neq c_{sv}$. We address these issues in §3.

We refer to this problem as "1-D," even though the covariance functions involve two spatial variables, and the saturation covariance has fluxes in both directions. The two variables represent two different points in the same 1-D domain. Similarly, the "2-D" problem has four spatial coordinates.

To define the vanishing-viscosity solution, first formally add the term $\epsilon_D \partial_x^2 s$ to (2.1) and carry out the expansion and derivation above. This adds diffusion terms $\epsilon_D \partial_x^2 \tilde{s}$, $\epsilon_D \partial_x^2 c_{sv}$, $\epsilon_D \partial_x^2 c_s$ to the right-hand sides of equations (2.9a), (2.9b), and (2.9c), respectively. Then find solutions in the limit $\epsilon_D \to 0$. In practice we solve the system (2.9) directly.

**2.3. Infinite expansion.** In this alternative derivation, flow variables head $h(x)$, velocity $v(x)$ and saturation $s(x,t)$ are represented by formal infinite perturbation series expansions in powers of a parameter $\epsilon$:

$$h = \sum_{n=0}^{\infty} \epsilon^n h_n(x), \qquad v = \sum_{n=0}^{\infty} \epsilon^n v_n(x), \qquad s = \sum_{n=0}^{\infty} \epsilon^n s_n(x,t). \tag{2.10}$$

The expansion parameter $\epsilon = \sigma_Y$ is shown to be appropriate within the context of the velocity and head equations (1.1) [7, pp. 184–190], [38]. For example, for single phase, stationary uniform mean flow in 1-D, $\sigma_v^2$ is approximated by $\epsilon^2 \langle v_1^2 \rangle = v_0^2 \sigma_Y^2$.

Moment equations analogous to (2.9) are derived in §A of the Appendix:

$$\partial_t s_0 + \partial_x \Big[ f(s_0) v_0 \Big] = 0, \qquad \partial_t \langle s_1 \rangle + \partial_x \Big[ v_0 f'(s_0) \langle s_1 \rangle \Big] = 0, \tag{2.11a}$$

$$\partial_t \langle s_2 \rangle + \partial_x \Big[ f(s_0) \langle v_2 \rangle + f'(s_0)\sigma_{sv} + f'(s_0) \langle s_2 \rangle v_0 + \frac{1}{2} f''(s_0)\sigma_s^2 v_0 \Big] = 0, \tag{2.11b}$$

$$\partial_t c_{sv} + \partial_x \Big[ f(s_0) c_v + f'(s_0) v_0 c_{sv} \Big] = 0, \tag{2.11c}$$

$$\partial_t c_s + \partial_x \Big[ f(s_0)\widehat{c}_{sv} + f'(s_0) v_0 c_s \Big] + \partial_y \Big[ f(s_0|_y) c_{sv} + f'(s_0|_y) v_0|_y c_s \Big] = 0. \tag{2.11d}$$

At $t = 0$, $s_0(x,0) = g(x)$, and $\langle s_1 \rangle (x,0)$, $\langle s_2 \rangle (x,0)$, $c_{sv}(x,y,0)$ and $c_s(x,y,0)$ are all zero. The second-order mean is $s_0 + \epsilon \langle s_1 \rangle + \epsilon^2 \langle s_2 \rangle$. Note that the argument of $f$ and its derivatives is $s_0$, the zeroth-order mean. The system is in fact closed again using a perturbation argument, but now this argument is contained in the assumption that the formal power series in $\epsilon$ converges. Thus, throughout §2, second-order equations are closed by assuming that heterogeneity is weak ($\sigma_Y \ll 1$).

**3. Classification of reduced equations.** Classification is of interest for several reasons. Notably, macrodispersion theories produce a parabolic equation for the mean. In contrast, our approach produces hyperbolic equations for mean and variance. To achieve this result, we exploit special structure in the equations in 1-D to simplify (2.9) and (2.11). First, we need the following

DEFINITION 3.1. *Let* $\mathbf{u}(x,y,t) : \mathbb{R}^2 \times \mathbb{R}_+ \to \mathbb{R}^n$, $\mathbf{F} : \mathbb{R}^n \to \mathbb{R}^n$, *and* $\mathbf{G} : \mathbb{R}^n \to \mathbb{R}^n$. *A system of equations in* conservation-law *form is given by*

$$\partial_t \mathbf{u} + \partial_x \mathbf{F}(\mathbf{u}) + \partial_y \mathbf{G}(\mathbf{u}) = 0, \quad \mathbf{u}(x,0) = \mathbf{u}_0(x). \tag{3.1}$$

*This system is* hyperbolic *if the eigenvalues of* $c_1\, DF(\mathbf{u}) + c_2\, DG(\mathbf{u})$ *are real for all* $c_1,\ c_2 \in \mathbb{R}$, *where* $DF$ *and* $DG$ *are the Jacobian matrices of* $\mathbf{F}$ *and* $\mathbf{G}$ [26].

We expect the equations to be nearly hyperbolic since the original deterministic PDE (1.2) is hyperbolic, but the systems (2.9) or (2.11) as given cannot even be written in conservation-law form due to the inconsistencies mentioned above. However, we show that both sets of MDEs reduce to hyperbolic systems of conservation laws and yield analytic solutions. The key discovery that allows this reduction is a relationship between covariance functions in 1-D.

Observe that velocity $\mathbf{v}$ is constant in 1-D, so it is merely a random variable rather than a random field. Thus, velocities at any two points in space are perfectly correlated (they are the same random variable). Equivalently, the velocity correlation length is infinite. This infinite correlation length characterizes the principal difference between stochastic subsurface flow in one and two space dimensions [18].

**3.1. Two-term expansion.** The MDEs (2.9) reduce to a system of hyperbolic PDEs. The first step to this end addresses the inconsistencies mentioned earlier.

Both expansion terms $\langle v \rangle$ and $\delta v$ are constant: by applying the expectation operator to $\partial_x v = 0$ we obtain $\partial_x \langle v \rangle = 0$, so that

$$0 = \partial_x v = \partial_x \langle v \rangle + \partial_x \delta v \quad \Rightarrow \quad \partial_x \delta v = 0. \tag{3.2}$$

This implies that $c_v(x,y)$ is also constant, and that $c_{sv}(x,y,t)$ is independent of its second argument. Consequently, $c_v$ is identical to the second-order approximation to velocity variance $\sigma_v^2$, and $c_{sv}(x,y,t)$ is identical to $\sigma_{sv}(x,t)$.

This last identity removes the inconsistency of having $\sigma_{sv}$ instead of $c_{sv}$. We still have $\sigma_s^2$ in (2.9a), instead of $c_s$, and we have $\langle s \rangle |_y$ and $\widehat{c}_{sv}$ in (2.9c). A key variance-covariance relationship, $\sigma_{sv} = \sigma_s\, \sigma_v$, follows: in 1-D, the saturation profile is completely determined by knowledge of the velocity, for any positive time. Thus, saturation and velocity are perfectly correlated. A generalization of this result is obtained directly from the MDEs in §3.3.

We divide (2.9b) by $\sigma_v > 0$, and retain only the first two equations in (2.9) in the following. Replace $c_v$ by $\sigma_v^2$ and $c_{sv}$ by $\sigma_v \sigma_s$, to reduce the system to the following new equations for mean and standard deviation of saturation:

$$\partial_t \begin{pmatrix} \langle s \rangle \\ \sigma_s \end{pmatrix} + \partial_x \begin{pmatrix} \langle v \rangle f(\langle s \rangle) + \sigma_v f'(\langle s \rangle)\sigma_s + \frac{1}{2} \langle v \rangle f''(\langle s \rangle)\sigma_s^2 \\ \sigma_v f(\langle s \rangle) + \langle v \rangle f'(\langle s \rangle)\sigma_s \end{pmatrix} = 0. \tag{3.3}$$

Dependence on the second space variable $y$ has been eliminated. Thus, (3.3) is in conservation-law form, with $\mathbf{u}(x,t) = (\langle s \rangle, \sigma_s)$, and flux function

$$\mathbf{F}(\mathbf{u}) = \begin{pmatrix} \langle v \rangle f(\langle s \rangle) + \sigma_v f'(\langle s \rangle)\sigma_s + \frac{1}{2} \langle v \rangle f''(\langle s \rangle)\sigma_s^2 \\ \sigma_v f(\langle s \rangle) + \langle v \rangle f'(\langle s \rangle)\sigma_s \end{pmatrix}. \tag{3.4}$$

LEMMA 1. *The MDEs* (2.9) *reduce to a hyperbolic system.*

*Proof.* It remains to show that (3.3) is strictly hyperbolic. The Jacobian matrix $DF(\langle s\rangle, \sigma_s) = \begin{pmatrix} j_{11} & j_{12} \\ j_{12} & j_{22} \end{pmatrix}$ has entries

$$\begin{aligned} j_{11} &= \langle v\rangle f'(\langle s\rangle) + \sigma_v f''(\langle s\rangle)\sigma_s + \frac{1}{2}\langle v\rangle f^{(3)}(\langle s\rangle)\sigma_s^2, \\ j_{12} &= \sigma_v f'(\langle s\rangle) + \langle v\rangle f''(\langle s\rangle)\sigma_s, \qquad j_{22} = \langle v\rangle f'(\langle s\rangle). \end{aligned} \tag{3.5}$$

$DF$ is symmetric; thus the eigenvalues of $DF$ are real and (3.3) is hyperbolic. In fact, we show that (3.3) is strictly hyperbolic; i.e., $DF$ has a complete set of linearly independent eigenvectors [26]. Distinct eigenvalues must correspond to independent eigenvectors. Thus, we need only consider the case where $DF$ has just one eigenvalue. This occurs when the discriminant of the characteristic polynomial vanishes: $(j_{11} - j_{22})^2 + 4j_{12}^2 = 0$. But this would imply that $j_{12} = 0$, hence $DF$ is a multiple of the identity, and again has a complete set of eigenvectors. The conclusion follows. □

In addition, the eigenvalues are distinct unless $(\langle s\rangle, \sigma_s) \in \{(0,0), (1,0)\}$ [18].

**3.2. Infinite expansion.** The evolution of moments in this case is given by the system (2.11). If velocity is constant then $v_j$ is constant for each $j$, so long as the perturbation series can be differentiated termwise. Thus, $c_v(x,y)$ is also constant, and $c_{sv}(x,y,t)$ is independent of its second argument. Consequently, $c_v$ is identical to the second-order approximation to velocity variance $\sigma_v^2$, and $c_{sv}(x,y,t)$ is identical to $\sigma_{sv}(x,t)$. Finally, the relationship $\sigma_{sv} = \sigma_v\,\sigma_s$ holds as before. Keeping only the first four equations in (2.11), replacing $c_v$ by $\sigma_v^2$ and $c_{sv}$ by $\sigma_v\sigma_s$, we obtain these equations analogous to (3.3):

$$\partial_t \begin{pmatrix} s_0 \\ \epsilon\langle s_1\rangle \\ \epsilon^2\langle s_2\rangle \\ \\ \sigma_s \end{pmatrix} + \partial_x \begin{pmatrix} v_0 f(s_0) \\ v_0 f'(s_0)\,\epsilon\langle s_1\rangle \\ \epsilon^2\langle v_2\rangle f(s_0) + \sigma_v f'(s_0)\sigma_s + v_0 f'(s_0)\,\epsilon^2\langle s_2\rangle \\ + \frac{1}{2}v_0 f''(s_0)\sigma_s^2 \\ \sigma_v f(s_0) + v_0 f'(s_0)\sigma_s \end{pmatrix} = 0. \tag{3.6}$$

We show that this system is (not strictly) hyperbolic. The Jacobian matrix $DF\left(s_0,\ \epsilon\langle s_1\rangle,\ \epsilon^2\langle s_2\rangle,\ \sigma_s\right) = \begin{pmatrix} d & 0 & 0 & 0 \\ j_{21} & d & 0 & 0 \\ j_{31} & 0 & d & j_{34} \\ j_{34} & 0 & 0 & d \end{pmatrix}$ has entries

$$\begin{aligned} &d = v_0 f'(s_0), \qquad j_{21} = v_0 f''(s_0)\epsilon\langle s_1\rangle, \qquad j_{34} = \sigma_v f'(s_0) + v_0 f''(s_0)\sigma_s, \\ &j_{31} = \epsilon^2\langle v_2\rangle f'(s_0) + \sigma_v f''(s_0)\sigma_s + v_0 f''(s_0)\epsilon^2\langle s_2\rangle + \frac{1}{2}v_0 f^{(3)}(s_0)\sigma_s^2. \end{aligned} \tag{3.7}$$

The spectrum of $DF$ consists of the single real eigenvalue $d$. Thus, the system (3.6) is hyperbolic, but not strictly hyperbolic. Furthermore, $DF$ in general does not have a full set of linearly independent eigenvectors (this occurs only when all off-diagonal elements are zero). This degeneracy of $DF$ leads to secular terms in the solution, which results in non-physical solutions. We show this explicitly in the next section. Use of the second-order mean as the argument of $f^{(k)}$ in §2.3 yields a modified infinite expansion that does not have this drawback, and is a fourth-order correction to the two-term expansion [18]. We will present a comparison of the modified expansion to the infinite and two-term expansions, and further analysis, in [19].

**3.3. Uniqueness, and an additional analytical result.** Because (2.9) and (2.11) are nearly hyperbolic systems, one might expect to extend uniqueness methods from the theory of such systems. The viscosity method is an appealing way to prove uniqueness [33]. We briefly outline the method below, which uses the vanishing-viscosity solution introduced in §1.1. Diffusive effects are generally present in the physical problem that is modeled by (3.1). Sharp profiles that evolve due to nonlinear advection are smoothed by diffusion, and solutions remain smooth for $t > 0$. Let $\mathbf{u}^\epsilon$ be the solution to the viscous form of (3.1) with diffusion coefficient (or "viscosity") $\epsilon_D > 0$. The viscous equation is

$$\partial_t \mathbf{u} + \partial_x \mathbf{F}(\mathbf{u}) + \partial_y \mathbf{G}(\mathbf{u}) = \epsilon_D(\partial_x^2 \mathbf{u} + \partial_y^2 \mathbf{u}). \tag{3.8}$$

It is generally thought to be easier to prove uniqueness for solutions to (3.8) than to (3.1) due to the regularizing effect of the diffusion operator $\epsilon_D(\partial_x^2 + \partial_y^2)$.

We seek the solution $\mathbf{u}^\epsilon$ to (3.8) in the limit $\epsilon_D \to 0$. If this limit exists and is unique in a suitable function space, we have the necessary result. Thus, we would like to carry out the following program:

1. Prove that (3.8) has a unique solution $\mathbf{u}^\epsilon$.
2. Prove that $\mathbf{u}^\epsilon$ has a unique limit in a suitably defined function space as $\epsilon_D \to 0$. Define the solution to (3.1) to be this limit.

Applying this or similar approaches to the problem of uniqueness for conservation law equations is found to be exceedingly difficult. It is usually applied only to *Riemann initial data*:

$$\mathbf{u} = \begin{cases} \mathbf{u}_l, & x < 0, \\ \mathbf{u}_r, & x > 0. \end{cases}$$

The states $\mathbf{u}_l$ and $\mathbf{u}_r$ are usually assumed to be "close" in some norm. The *Riemann problem* that consists of a hyperbolic PDE in conservation-law form with Riemann initial data is the fundamental Cauchy problem for this class of equations [33].

Variations on the viscosity method have been used for 1-D conservation laws with some success. The result for scalar equations was obtained by Oleinik (cited in [33]), and was extended to some systems of two equations (see [5] for a recent result and additional references). Uniqueness proofs for systems of equations are generally limited to *genuinely nonlinear* or *linearly degenerate* equations [33]. Neither the deterministic version of equation (2.1) nor the reduced systems above possess either of these properties. A review of the literature does not reveal a result general enough to guarantee uniqueness for (2.9). Thus uniqueness remains an open question; however, physical and mathematical arguments suggest that such results can eventually be obtained. For now, we must be satisfied with

CONJECTURE 3.1 (uniqueness). *Moment equations* (2.9) *or* (2.11) *have at most one vanishing-viscosity solution for uniformly bounded, measurable initial data.*

Now we obtain a more general form of the covariance relationship stated in §§3.1–3.2 directly from the MDEs.

LEMMA 2. *If there exists a unique solution to* (2.9) *with bounded, measurable initial data, then*

$$c_s\, c_v = c_{sv}\, \widehat{c}_{sv}. \tag{3.9}$$

*The same holds for* (2.11).

*Proof.* We prove (3.9) for (2.9) in the sense of vanishing viscosity. The proof for (2.11) is nearly identical. Adding a linear diffusion term $-\partial_x(\epsilon_D \partial_x s)$ to the left-hand side of (2.1) with $\epsilon_D > 0$ deterministic, we obtain the viscous form of the covariance equations

$$\partial_t c_{sv} + \partial_x \Big[ f(\langle s \rangle) c_v + f'(\langle s \rangle) v_0 c_{sv} - \epsilon_D \partial_x c_{sv} \Big] = 0, \tag{3.10}$$

$$\partial_t c_s + \partial_x \Big[ f(\langle s \rangle) \widehat{c}_{sv} + f'(\langle s \rangle) v_0 c_s - \epsilon_D \partial_x c_s \Big] + \partial_y \Big[ f(\langle s \rangle|_y) c_{sv} + f'(\langle s \rangle|_y) v_0|_y c_s - \epsilon_D \partial_y c_s \Big] = 0. \tag{3.11}$$

Once the identity is proven for (3.10) and (3.11), we formally let $\epsilon_D \to 0$.

Multiply (3.10) by $\widehat{c}_{sv}$ and add to $c_{sv}$ times the corresponding equation for $\widehat{c}_{sv}$. Apply the identity $\widehat{c}_{sv}\, \partial_t c_{sv} + c_{sv}\, \partial_t \widehat{c}_{sv} = \partial_t(\widehat{c}_{sv}\, c_{sv})$. Note that $\widehat{c}_{sv}$ is independent of $x$. We obtain

$$\partial_t(\widehat{c}_{sv}\, c_{sv}) + \partial_x \Big[ f(\langle s \rangle) c_v\, \widehat{c}_{sv} + f'(\langle s \rangle) v_0 (c_{sv}\, \widehat{c}_{sv}) - \epsilon_D \partial_x (c_{sv}\, \widehat{c}_{sv}) \Big] + \partial_y \Big[ f(\langle s \rangle|_y) c_v\, c_{sv} + f'(\langle s \rangle|_y) v_0|_y (c_{sv}\, \widehat{c}_{sv}) - \epsilon_D \partial_x (c_{sv}\, \widehat{c}_{sv}) \Big] = 0. \tag{3.12}$$

This equation is identical to (3.11), scaled by $c_v$. Both $c_v\, c_s$ and $c_{sv}\, \widehat{c}_{sv}$ are initially zero. The identity (3.9) follows by letting $\epsilon_D \to 0$ and recalling the uniqueness hypothesis. □

Again $\sigma_{sv} = \sigma_s\, \sigma_v$ follows by letting $y \to x$ so that $c_s \to \sigma_s^2$, and $\widehat{c}_{sv} \to \sigma_{sv}$. It is important to recognize that this covariance relationship follows from observation. The fact that it is also a consequence of the MDEs (subject to uniqueness) shows that the MDEs are consistent with this intuitive result.

**4. Solution.** We present results for the linear advection case first, then a solution for nonlinear advection with the two-term expansion.

**4.1. Linear advection.** We solve (3.3) and (3.6) for $f(s) = s$ with deterministic initial data $s(x,0) = g(x) \in \mathcal{C}^1$. These easily obtained results exhibit bimodal behavior similar to the nonlinear case. This linear flux case represents pure advection of conservative solute transport in single-phase flow, with $s$ as solute concentration. We also show that moments given by the infinite expansion violate physical bounds.

**4.1.1. Two-term expansion.** With $f(s) = s$, (3.3) becomes

$$\partial_t \begin{pmatrix} \langle s \rangle \\ \sigma_s \end{pmatrix} + \begin{pmatrix} \langle v \rangle & \sigma_v \\ \sigma_v & \langle v \rangle \end{pmatrix} \partial_x \begin{pmatrix} \langle s \rangle \\ \sigma_s \end{pmatrix} = 0, \tag{4.1}$$

with initial data $\langle s \rangle (x,0) = g(x)$ and $\sigma_s(x,0) = 0$. The eigenvalues of the Jacobian matrix, representing wave speeds, are $\lambda_1 = \langle v \rangle - \sigma_v$ and $\lambda_2 = \langle v \rangle + \sigma_v$. The solution is given by

$$\langle s \rangle(x,t) = \frac{1}{2}\left[ g(x - \lambda_2 t) + g(x - \lambda_1 t) \right], \quad \sigma_s(x,t) = \frac{1}{2}\left[ g(x - \lambda_2 t) - g(x - \lambda_1 t) \right]. \tag{4.2}$$

Each moment is a superposition of waves that move at distinct speeds $\lambda_1 < \lambda_2$. Figure 4.1 shows mean saturation for a Gaussian initial profile. The peaks of the two modes separate at a speed of $\lambda_2 - \lambda_1 = 2\sigma_v\, t$. We used the following standard results for uniform mean flow, $x \in [0, L]$, with stationary log hydraulic conductivity ($\langle Y \rangle$ and $\sigma_Y$ do not depend on $x$) [7, 14]:

$$\langle v(x) \rangle = \frac{K_G J}{\phi}\left(1 - \frac{\sigma_Y^2}{2}\right), \qquad \sigma_v^2 = \left(\frac{K_G J}{\phi}\right)^2 \sigma_Y^2, \tag{4.3}$$

where $K_G = \exp(\langle Y \rangle)$ and $J$ is the negative mean head gradient. We used parameters $K_G\, J = 0.5$, $\phi = 0.2$, and $\sigma_Y = 0.5$.

This is a non-physical result; we do not expect an initial localized solute pulse to evolve into a bimodal mean profile. Adding a linear diffusion term to (4.1) will not eliminate this bimodality; in this situation, separation between modes will not be observed immediately, but will eventually appear due to a separation speed that is linear in time. This is evident in the nonlinear case (§4.3), where numerical and artificial diffusion are present in our numerical scheme, but the two-wave character is clearly seen.

**4.1.2. Infinite expansion.** Moment equations (3.6) with $f(s) = s$ are

$$\partial_t \begin{pmatrix} s_0 \\ \epsilon^2 \langle s_2 \rangle \\ \sigma_s \end{pmatrix} + \begin{pmatrix} v_0 & 0 & 0 \\ \epsilon^2 \langle v_2 \rangle & v_0 & \sigma_v \\ \sigma_v & 0 & v_0 \end{pmatrix} \partial_x \begin{pmatrix} s_0 \\ \epsilon^2 \langle s_2 \rangle \\ \sigma_s \end{pmatrix} = 0. \tag{4.4}$$

The equation for $\langle s_1 \rangle$ is not needed, since $\langle s_1 \rangle \equiv 0$. Each equation can be solved separately, in the sequence $s_0$, $\sigma_s$, $\epsilon^2 \langle s_2 \rangle$ to obtain

$$\begin{aligned} s_0(x,t) = g(x - v_0 t), \quad \sigma_s(x,t) = -\sigma_v t g'(x - v_0 t), \\ \epsilon^2 \langle s_2 \rangle (x,t) = -\epsilon^2 \langle v_2 \rangle\, t\, g'(x - v_0 t) + \frac{\sigma_v^2}{2} t^2 g''(x - v_0 t). \end{aligned} \tag{4.5}$$

The prime ($'$) indicates a derivative with respect to the argument $z = x - v_0 t$ of the function $g(z)$. The second-order approximation to mean saturation is given by $\langle s \rangle \approx \tilde{s} \equiv s_0 + \epsilon^2 \langle s_2 \rangle$.

The term $\frac{\sigma_v^2}{2} t^2 g''(x - v_0 t)$ will dominate this approximation to $\langle s \rangle$ for large time, if $g''$ is not identically zero. Thus the magnitude of the approximation can grow without bound. An example for a Gaussian initial profile is shown in figure 4.1. Here again, we use a standard result for uniform mean flow with stationary log conductivity [38] giving $v_0 = K_G\, J/\phi$, $\epsilon^2 \langle v_2 \rangle = -v_0\, \sigma_Y^2/2$, and $\sigma_v = v_0\, \sigma_Y$, and parameters are the same as in §4.1.1. The mean behavior is similar for two-term and infinite expansions; the result in the latter is evidently worse because it violates physical bounds on mean saturation (saturation must remain between 0 and 1). This renders the infinite expansion inappropriate. It is clear from (4.2) that the mean always lies within physical bounds for the two-term expansion. For the nonlinear flux case, we study the two-term expansion only.

REMARK 4.1. Bimodal mean concentration (or saturation, in our case) was noted in [21], [24] and [25]. All used methods to derive mean transport equations that do not involve second-order corrections. In [21], Koch and Brady model the concentration–velocity covariance using a spectral method, and show that the equation for mean concentration has a wave-like character with two wave speeds. They point out that the bimodality is most pronounced as the velocity correlation length tends to $\infty$, to which they refer as the "most anomalous case". This is the case in one dimension, as noted above.

In [24, 25], Lenormand and Wang derive a mean transport equation representing an ensemble of transport in streamlines. One version of their equation is derived from a series expansion of a Fourier transform, truncated at second *temporal* moments. For an example of layered material, this equation is shown to have the wave character as in [21], and it is suggested that bimodality may be eliminated by incorporating higher-order temporal moments. If this is indeed the case, it may suggest that incorporating

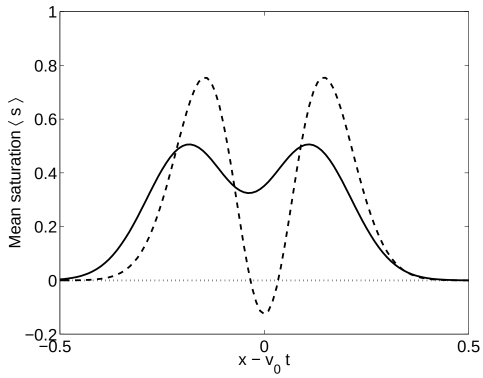


FIG. 4.1. *Mean saturation, linear flux with Gaussian initial profile for uniform mean flow. Both two-term (solid) and infinite expansion (dotted) moments exhibit bimodal behavior. The latter violates physical bounds on saturation.*

higher-order statistical moments in our equations eliminates bimodality. However, when higher moments are retained in the mean equation, equations for these moments must also be generated. The system of equations expands very quickly as higher moments are incorporated.

**4.2. Nonlinear advection.** Equation (3.3) is in the form (3.1) with $\mathbf{G} \equiv 0$. For nonlinear $\mathbf{F}(\mathbf{u})$, a solution consists of a sequence of shock waves, constant states, and rarefaction waves. We begin by briefly reviewing some of the theory of hyperbolic systems of conservation laws. Several details are omitted and can be found in [29, 33].

**4.2.1. Rarefactions.** Rarefaction waves are self-similar solutions in $\mathcal{C}^1$ that depend on the similarity variable $\eta = x/t$ only. Let $\mathbf{u} = \mathbf{u}(\eta)$; then (3.1) implies that

$$-\eta \frac{d\mathbf{u}}{d\eta} + DF(\mathbf{u})\, \frac{d\mathbf{u}}{d\eta} = 0, \tag{4.6}$$

where $DF(\mathbf{u})$ is the Jacobian matrix of $\mathbf{F}(\mathbf{u})$. Let the eigenvalues of $DF(\mathbf{u})$ be ordered $\lambda_1(\mathbf{u}) \leq \lambda_2(\mathbf{u})$ and let $\mathbf{r}_k(\mathbf{u})$ be the associated eigenvectors ($k = 1, 2$). Then $\eta$ must be an eigenvalue $\lambda_k(\mathbf{u})$ and $d\mathbf{u}/d\eta$ is proportional to the eigenvector $\mathbf{r}_k(\mathbf{u})$. This relationship is given explicitly as

$$\frac{d\mathbf{u}}{d\eta} = \big(\nabla\lambda_k(\mathbf{u}) \cdot \mathbf{r}_k(\mathbf{u})\big)^{-1} \mathbf{r}_k(\mathbf{u}) \tag{4.7}$$

for each $k$, and is valid as long as the directional derivative $\nabla\lambda_k(\mathbf{u}) \cdot \mathbf{r}_k(\mathbf{u})$ does not vanish. It follows that these waves are integral curves of the vector fields defined by eigenvectors of $DF$ in the phase plane defined by $\mathbf{u}$. The integral curves must have eigenvalues increasing in $\eta$; otherwise, characteristics cross and new shocks form. The most general theory for hyperbolic systems requires that the system be either *genuinely nonlinear* ($\nabla\lambda_k \cdot \mathbf{r}_k \neq 0$) or *linearly degenerate* ($\nabla\lambda_k \cdot \mathbf{r}_k \equiv 0$) [4, 29, 33].

**4.2.2. Weak solutions, shocks, and entropy conditions.** Shocks are allowed if we consider the weak form of (3.1). Let the shock be defined in the $(x, t)$ plane by $x = \xi(t)$; its speed is given by $\dot{\xi} \equiv d\xi/dt$. Let $\mathbf{u}^-$ and $\mathbf{u}^+$ be the solution values to the left and right (along the $x$-axis) of the shock. Then the *Rankine–Hugoniot* condition is given by

$$[\mathbf{u}^+ - \mathbf{u}^-]\dot{\xi}(t) = [\mathbf{F}(\mathbf{u}^+) - \mathbf{F}(\mathbf{u}^-)]. \tag{4.8}$$

*Entropy conditions* are then imposed to capture the vanishing-viscosity solution to (3.1). For scalar hyperbolic equations, this requirement is sufficient: the vanishing-viscosity solution is identical to the weak solution that satisfies an entropy condition. Since this issue is directly related to the question of uniqueness, such a statement cannot yet be made for (3.1) in general. We apply the following well-known entropy condition.

DEFINITION 4.1 (Lax condition). *A shock connecting the states* $\mathbf{u}^-$ *and* $\mathbf{u}^+$*, traveling with speed* $\dot{\xi}$ *is admissible if*

$$\lambda_k(\mathbf{u}^+) \leq \dot{\xi} \leq \lambda_k(\mathbf{u}^-) \tag{4.9}$$

*for one of the characteristic speeds* $\lambda_k$*,* $k = 1, 2$*.*

In words, the *characteristic curves* defined by $dx/dt = \lambda_k(\mathbf{u})$ must run into the shock, not out of it, as $t$ increases [33]. A solution in the phase plane is a connected set of rarefaction and shock curves that satisfy the Lax condition. However, in our case it is not enough to simply apply (4.6)–(4.9). As we present our solution, we introduce an additional entropy condition due to Liu [27–29] to address the specific structure of our equations.

**4.3. Moment Equations.** Now we present a solution to the MDEs (3.3) for nonlinear $f(s)$ that satisfies entropy conditions. For illustration we choose $f(s) = s^2/(s^2 + m(1-s)^2)$ with *viscosity ratio* $m = 1/2$. We consider deterministic initial saturation given by the Heaviside function $s(x, 0) = H[-x]$, so that $\sigma_s$ is initially zero. This models an oil-saturated reservoir with water forced in at the origin (we assume $v > 0$). To simplify notation of (3.3), set $u_1 = \langle s \rangle$, $u_2 = \sigma_s$, and $\tau = \langle v \rangle\, t$ so that $\partial_t = \langle v \rangle\, \partial_\tau$. Let $\epsilon \equiv \sigma_v / \langle v \rangle$ (this is consistent with the $\epsilon$ previously used as an expansion parameter). The scaled equations are

$$\partial_\tau \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} + \partial_x \begin{pmatrix} f + \epsilon f' u_2 + \frac{1}{2} f'' u_2^2 \\ \epsilon f + f' u_2 \end{pmatrix} = 0. \tag{4.10}$$

Note that the argument of $f$ and its derivatives is always $u_1$. Let $\mathbf{u} = (u_1, u_2)$. The Jacobian matrix is

$$DF(\mathbf{u}) = \begin{pmatrix} f' + \epsilon f'' u_2 + \frac{1}{2} f^{(3)} u_2^2 & \epsilon f' + f'' u_2 \\ \epsilon f' + f'' u_2 & f' \end{pmatrix}. \tag{4.11}$$

¿From §3.1 we know that the eigenvalues of $DF$ are real and may be ordered $\lambda_1 < \lambda_2$ except at $\mathbf{u} \in \{(0,0), (1,0)\}$, where both are zero. The corresponding eigenvectors are $\mathbf{r}_k(\mathbf{u})$, $k = 1, 2$.

The true mean and standard deviation of saturation must be non-negative. The mean cannot exceed unity, as it represents a fraction. Therefore, we only consider the subdomain $\mathbf{u} \in [0,1] \times [0, \infty)$ of the phase plane. The endpoints of the solution to (4.10) are $\mathbf{u} = (1,0)$ and $\mathbf{u} = (0,0)$, which represent a boundary condition, and the initial condition for positive $x$, respectively.

Vector fields $\mathbf{r}_k(\mathbf{u}(\eta))$ are shown in figure 4.2, pointing in the direction of increasing eigenvalue ($\nabla\lambda_k \cdot \mathbf{r}_k > 0$). To obtain a rarefaction curve, one solves (4.7) for given initial data for a single $k$ value. Moving in the direction of increasing $\eta$, a rarefaction continues so long as $\nabla\lambda_k \cdot \mathbf{r}_k > 0$. An *inflection locus* [17], consisting of points where $\nabla\lambda_k \cdot \mathbf{r}_k = 0$, can be inferred from figure 4.2 where vectors reverse direction. This locus of curves represents a barrier to rarefactions. The existence of the inflection locus is evidence that the system is neither genuinely nonlinear nor linearly degenerate.

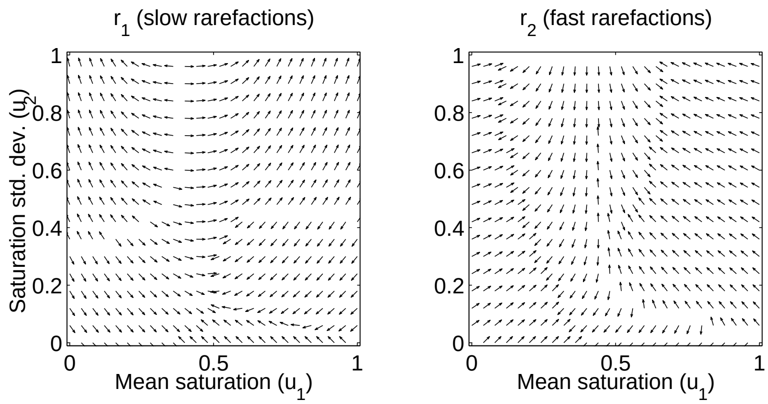


FIG. 4.2. *Slow and fast rarefaction vector fields.*

The steps to a solution are similar to those in the deterministic case, which is reviewed for comparison in §B. We first study the behavior near the boundary value $\mathbf{u} = (1, 0)$, and follow the solution forward in $\eta = x/\tau$. When $\epsilon = 0$, this is just the scalar deterministic case, which has a rarefaction connecting to $s = 1$. Thus, we expect a rarefaction to connect to $(1, 0)$. We find that only a slow rarefaction, corresponding to $\lambda_1$ and designated $R_1(\eta)$, may connect to $(1, 0)$ (see figure 4.3). This curve is continued from $(1, 0)$ to a point $\mathbf{u}^*$ just short of the inflection locus.

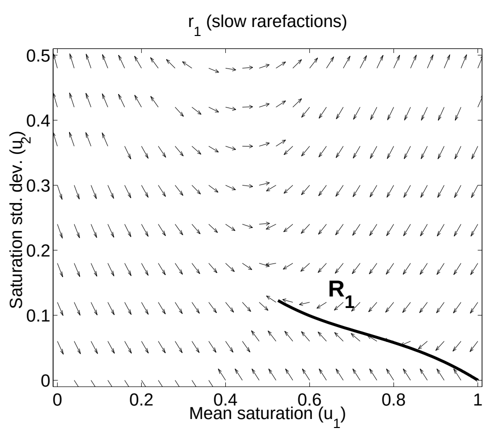


FIG. 4.3. *Construction of the slow rarefaction* $R_1$ *from* $(1, 0)$.

Next, consider the solution near $(0, 0)$, the "end" value of $\mathbf{u}$ on the right (in $x$). We find that a shock must connect to this point, as in the deterministic case. The point $(0, 0)$ lies to the right (in $x$) of the shock, so let $\mathbf{u}^+ = (u_1^+, u_2^+) = (0, 0)$. All points $\mathbf{u} = (u_1, u_2)$ on a possible shock curve connecting to $u^+$ are defined by (4.8) as follows:

$$
\begin{aligned}
(u_1^+ - u_1)\,\dot{\xi} &= F_1(\mathbf{u}^+) - F_1(\mathbf{u}) \\
(u_2^+ - u_2)\,\dot{\xi} &= F_2(\mathbf{u}^+) - F_2(\mathbf{u}),
\end{aligned} \tag{4.12}
$$

where

$$
\begin{aligned}
F_1(\mathbf{u}) &= f(u_1) + \epsilon f'(u_1)u_2 + \frac{1}{2} f''(u_1)u_2^2, \\
F_2(\mathbf{u}) &= \epsilon f(u_1) + f'(u_1)u_2
\end{aligned} \tag{4.13}
$$

(from (4.10)). Eliminating $\dot{\xi}$ in (4.12) gives an implicit definition of the curve on which points $\mathbf{u}$ lie, and we may write this definition formally as $\Phi(\mathbf{u};\, \mathbf{u}^+) = 0$. This gives a continuous set of possible $\mathbf{u}$, speeds $\dot{\xi}$, and eigenvalues $\lambda_k(\mathbf{u})$. We follow this curve from the starting point $\mathbf{u}^+$ as long as the Lax entropy condition (4.9) is satisfied, which is tested by computing the speed $\dot{\xi}$ using (4.12), and the eigenvalues $\lambda_k$ at each point $\mathbf{u}$. The Lax condition in this case is

$$
\lambda_k(\mathbf{u}^+) \le \dot{\xi} \le \lambda_k(\mathbf{u}). \tag{4.14}
$$

The point $\mathbf{u}^-$ to the left (in $x$) of the shock is the endpoint of this curve in the phase plane. In addition, the following criterion must be met [27, 29].

DEFINITION 4.2 (Liu Criterion). *Define the Hugoniot curves*

$$
H_k(\mathbf{u}_0) = \{\mathbf{u} : (\mathbf{u} - \mathbf{u}_0)\varsigma = \mathbf{F}(\mathbf{u}) - \mathbf{F}(\mathbf{u}_0)\}, \quad k = 1, 2
$$

*for some scalar* $\varsigma = \varsigma(\mathbf{u}_0, \mathbf{u})$. *The shock conditions* (4.14) *tell us that* $\mathbf{u}^+ \in H_k(\mathbf{u}^-)$ *and* $\dot{\xi} = \varsigma(\mathbf{u}^-, \mathbf{u}^+)$. *A shock with speed* $\dot{\xi} = \varsigma(\mathbf{u}^-, \mathbf{u}^+)$ *is admissible if it satisfies*

$$
\dot{\xi} = \varsigma(\mathbf{u}^-, \mathbf{u}^+) \le \varsigma(\mathbf{u}^-, \mathbf{u}) \tag{4.15}
$$

*for any* $\mathbf{u} \in H_k(\mathbf{u}^-)$ *between* $\mathbf{u}^-$ *and* $\mathbf{u}^+$.

In general, two curves may pass through each point $\mathbf{u}^+$ and satisfy $\Phi(\mathbf{u};\, \mathbf{u}^+) = 0$ [29, 33], but only one continues from $(0, 0)$ into the first quadrant. This curve is shown on the left in figure 4.4 along with $R_1$. At each point on the curve, $\lambda_1(\mathbf{u}) < \dot{\xi} \le \lambda_2(\mathbf{u})$, so it is a "2-shock". We designate this curve $S_2$ and its speed $\dot{\xi}_2$. Points along this curve are admissible as long as (4.14) and (4.15) are satisfied for $k = 2$. Notice that this curve crosses the inflection locus for $\lambda_2$.

Evidently, an intermediate solution between $R_1$ and $S_2$ is necessary. A slow rarefaction cannot continue on to meet $S_2$, and we find that a fast rarefaction curve cannot connect the two curves. The connection must involve a shock; the simplest possibility is a single slow shock. We follow a possible shock forward in $\eta = x/\tau$ from points on $R_1$. This leads to an admissible solution, if we account for the following. We know that the intermediate shock, designated $S_1$ with speed $\dot{\xi}_1$, must satisfy the entropy condition $\lambda_1(\mathbf{u}^+) \le \dot{\xi}_1 \le \lambda_1(\mathbf{u}^-)$, and the condition (4.15). But since $S_1$ connects to a rarefaction on the left (in $x$), we must have $\lambda_1(\mathbf{u}^-) = \dot{\xi}_1$. Otherwise, the value $\mathbf{u}^-$ to the left of the shock travels faster than the shock front, which is not allowed. Thus, we find the point at which $R_1$ connects to $S_1$ by matching rarefaction and shock speeds at the front.

An algorithm for the speed-matching step for the MDEs is provided in §C of the Appendix. By following a shooting procedure outlined in that algorithm, we obtain an approximation to a curve labelled $S_1$ which connects $R_1$ to $S_2$, shown on the right in figure 4.4. The condition (4.15) is also satisfied for $S_1$ at the end of this process.

The solution in physical space is pieced together from the phase space solution as follows. Fix $\tau = \langle v \rangle\, t$. Along $R_1$, the location is computed by $x = \lambda_1(\mathbf{u})\,\tau$, for

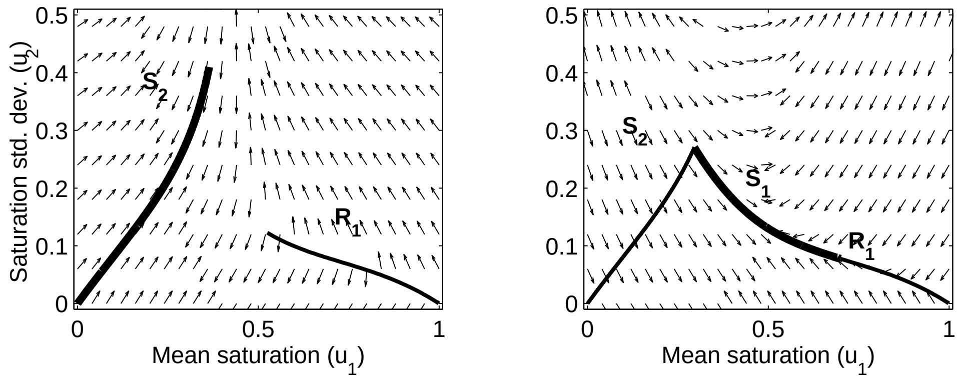


FIG. 4.4. *Construction of shocks connecting to rarefaction $R_1$ and $(0,0)$. First, a fast shock $S_2$ connecting to $(0,0)$ is constructed. Then a slow shock is introduced to connect $R_1$ and $S_2$. "Fast" and "slow" vector fields $\mathbf{r}_2$ and $\mathbf{r}_1$ are illustrated in the left and right plots, respectively.*

$\mathbf{u}$ between $\mathbf{u}^-$ and $(1,0)$. $R_1$ and $S_1$ connect at $\mathbf{u}^-$, where $x^{(1)} \equiv \dot{\xi}_1 \tau = \lambda_1(\mathbf{u}^-)\tau$. The solution is constant from $x^{(1)}$ to $x^{(2)} \equiv \dot{\xi}_2 \tau$, where it then jumps to zero. This solution is compared to the solution obtained from our numerical PDE scheme in figure 4.5, for $L=2$, $m=1/2$, $\langle v \rangle = 5/2$, $\sigma_v = 5/4$ at a fixed time $t=0.2$.

We have a solution that satisfies entropy conditions, but uniqueness of the solution is not resolved. Most results, again, require genuine nonlinearity or linear degeneracy, and our system does not satisfy these conditions. Liu extended existence and uniqueness results to more general systems [27, 28], but the restrictions he places on flux functions are not met by $F_1$ and $F_2$, and most results require "small data" (that is, a small jump $\|\mathbf{u}^- - \mathbf{u}^+\|$; see [5] for one extension to "large data").

However, it is clear in figure 4.5 that this solution matches that obtained from a numerical PDE scheme applied directly to (4.10). Our first-order upwind PDE scheme includes numerical and artificial diffusion. The diffusion coefficient is roughly three orders of magnitude smaller than the jumps in solution values. Thus the numerical solution is near the vanishing-viscosity limit. The numerical result also shows that the addition of linear diffusion terms does not eliminate bimodality in the solution.

The saturation variance is supported primarily on an uncertainty interval between fronts. Physically, the solution represents two zones containing mixtures of the two fluid phases (for example, water and oil), and a third containing only the oil phase. In the first zone, we have a smoothly varying mixture from the injection boundary $(x=0)$, where the mean oil content tends to zero, down to a constant mixture just left of a shock. In the second zone, we have a constant mix of oil and water. The solution does not represent physical reality. Rather than two shock waves, the true mean saturation is more likely to have a smooth, diffuse profile. Taken with the profile of $\sigma_s$, however, these second-order solutions provide some insight into the propagation of uncertainty in two-phase flow.

In the limit $\sigma_Y \to 0$ the mean saturation tends to the classic Buckley–Leverett profile in figure B.1. The analogous construction of a solution in the scalar deterministic saturation case (§B) can now be stated succinctly. In that case, the initial rarefaction is followed forward in $x$, up to the inflection point $f''(s^*)=0$. A shock connects to the rarefaction from $s^+=0$ to $s^- > s^*$, where the shock speed matches the characteristic speed $v\, f(s^-)/s^- = v\, f'(s^-)$.

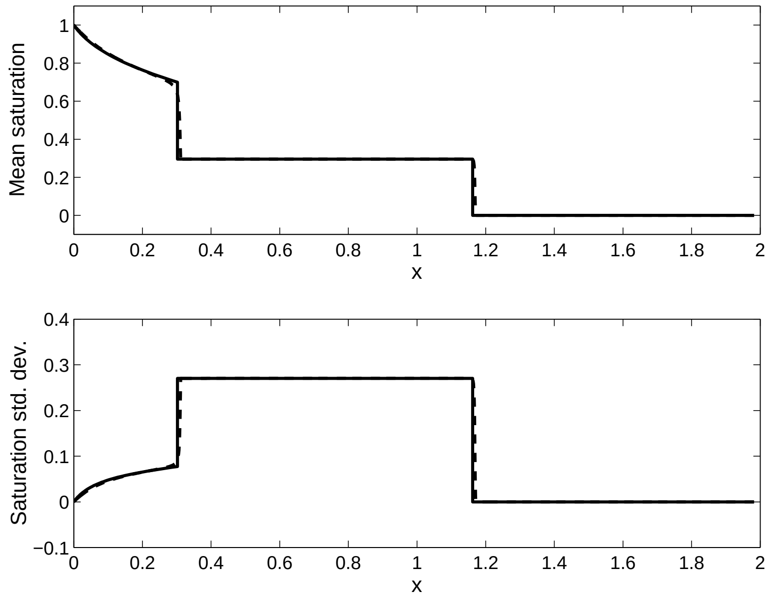


FIG. 4.5. *Mean and standard deviation of saturation. The solid curve is obtained from semi-analytical construction of shocks and rarefaction curves in phase space; dashed curve is obtained from numerical PDE scheme applied directly to* (4.10).

For our semi-analytical solution described above, the approximation to $R_1$ was obtained with an explicit Runge-Kutta (4,5) formula (function `ode45`) in MATLAB®. Shock curves were approximated by incrementing $u_1$, and solving for $u_2$ using the `roots` function in MATLAB.

**5. Conclusions.** For spatial resolution of uncertainty, these bimodal results suggest that second-order Eulerian MDEs may be inappropriate for 1-D immiscible flow. Unlike 1-D, $\mathbf{v}$ has finite correlation length in 2-D, and macrodispersion models are based on correlations in $\delta\mathbf{v}$. In results for analogous MDEs for passive 2-D solute transport with diffusion, bimodality was not observed [15]; one might expect macrodispersion to lead to a similar result for immiscible flow. Nevertheless, in a forthcoming submission we show that somewhat mitigated bimodality does persist in 2-D, even with diffusion terms [20]. More positively, for spatial averages such as oil-production curves, good matches to Monte Carlo simulations are found.

**6. Acknowledgments.** Ken Jarman would like to thank Joseph Oliveira for many helpful suggestions and invaluable guidance through extensive conversations.

**Appendix A. Moment equations for infinite expansion.**

We derive equations for moments of saturation and velocity using the asymptotic series in (2.10). Moments of $\ln K$, $h$, and $v$ are known. A note on terminology is appropriate. The term "order" applies to the power of $\epsilon$, rather than the order of the statistical moment. In special cases we may use the term "order" in the latter sense and clearly differentiate from order in $\epsilon$. Thus, a "second moment" is a covariance, but "second-order moment" is any moment that is approximated to order $\epsilon^2$.

Expand $f(s)$ in a Taylor series around $s_0(x,t)$:

$$\begin{aligned} f(s) &= f(s_0) + f'(s_0)(s-s_0) + \frac{1}{2}f''(s_0)(s-s_0)^2 + \cdots \\ &= f(s_0) + f'(s_0)\big(\epsilon(s_1 - \langle s_1\rangle) + \epsilon^2(s_2 - \langle s_2\rangle) + \epsilon^3 s_3 + \cdots\big) \\ &\quad + \frac{1}{2}f''(s_0)\big(\epsilon(s_1 - \langle s_1\rangle) + \epsilon^2(s_2 - \langle s_2\rangle) + \epsilon^3 s_3 + \cdots\big)^2 + \cdots . \end{aligned} \tag{A.1}$$

Applying this expansion to (2.1) obtains the zeroth- and first-order equations

$$\partial_t s_0 + \partial_x[f(s_0)v_0] = 0, \tag{A.2}$$

$$\partial_t s_1 + \partial_x\Big[f(s_0)v_1 + f'(s_0)s_1 v_0\Big] = 0. \tag{A.3}$$

Observe that $\langle s_0\rangle = s_0$ since all terms in the equation for $s_0$ are deterministic. From the theory of MDEs of single phase flow we find that $\langle v_1\rangle = 0$ [41], so that applying the operator $\langle\cdot\rangle$ to (A.3) gives

$$\partial_t \langle s_1\rangle + \partial_x\Big[v_0 f'(s_0)\langle s_1\rangle\Big] = 0, \tag{A.4}$$

with initial data $\langle s_1\rangle(x,0) = 0$.

PROPOSITION 3. *Where* (A.2) *and* (A.4) *admit solutions* $s_0, \langle s_1\rangle$ *in* $\mathcal{C}^1$, $\langle s_1\rangle = 0$.

*Proof.* Solutions in $\mathcal{C}^1$ are self-similar, with similarity variable $\eta = x/t$. Substituting $s_0(\eta)$ into (A.2) gives

$$v_0 f'(s_0(\eta)) = \eta$$

Using this identity and substituting $\langle s_1\rangle = \langle s_1\rangle(\eta)$ into (A.4) gives

$$\begin{aligned} 0 &= \partial_t\langle s_1\rangle + \partial_x[\eta\langle s_1\rangle] \\ &= \partial_\eta\langle s_1\rangle\frac{\partial\eta}{\partial t} + \partial_\eta[\eta\langle s_1\rangle]\frac{\partial\eta}{\partial x} \\ &= -\frac{\eta}{t}\partial_\eta\langle s_1\rangle + \frac{\eta}{t}\partial_\eta\langle s_1\rangle + \frac{1}{t}\langle s_1\rangle, \end{aligned}$$

and the proposition follows. □

We conjecture that $\langle s_1\rangle = 0$ for discontinuous solutions as well. Applying $\langle\cdot\rangle$ to the second-order equation gives the following:

$$\partial_t\langle s_2\rangle + \partial_x\Big[f(s_0)\langle v_2\rangle + f'(s_0)\langle s_1 v_1\rangle + f'(s_0)\langle s_2\rangle v_0 + \frac{1}{2}f''(s_0)\langle {s_1}^2\rangle v_0\Big] = 0. \tag{A.5}$$

Now we derive equations for second moments. Multiply the first-order equation (A.3) by $v_1(y)$ and apply $\langle\cdot\rangle$ to obtain the equation for the two-point saturation-velocity covariance,

$$\partial_t\langle s_1 v_1|_y\rangle + \partial_x\Big[f(s_0)\langle v_1 v_1|_y\rangle + f'(s_0)v_0\langle s_1 v_1|_y\rangle\Big] = 0. \tag{A.6}$$

Similarly, multiply (A.3) by $s_1(y,t)$ and apply $\langle\cdot\rangle$ to obtain the equation for the two-point saturation covariance,

$$\begin{aligned} &\partial_t\langle s_1 s_1|_y\rangle + \partial_x\Big[f(s_0)\langle s_1|_y v_1\rangle + f'(s_0)v_0\langle s_1 s_1|_y\rangle\Big] \\ &\qquad + \partial_y\Big[f(s_0|_y)\langle s_1 v_1|_y\rangle + f'(s_0|_y)v_0|_y\langle s_1|_y s_1\rangle\Big] = 0. \end{aligned} \tag{A.7}$$

The system for this version consists of the moment equations (A.2) and (A.4)–(A.7). Defining $c_{sv}(x,y,t) = \langle s_1 v_1|_y\rangle$, $c_s = \langle s_1 s_1|_y\rangle$, $c_v = \langle v_1 v_1|_y\rangle$, and $\widehat{c}_{sv}(x,y,t) = c_{sv}(y,x,t)$, the system is given by (2.11). If the conjecture that $\langle s_1\rangle = 0$ holds, then it is not necessary to include (A.4).

**Appendix B. Deterministic Buckley–Leverett.** When $\sigma_Y \to 0$, (2.1) and (3.3) reduce to a deterministic Buckley–Leverett model:

$$\partial_t s + \partial_x (f(s)v) = 0, \tag{B.1}$$

with initial data $s(x,0) = H[-x]$ as in §4.3. Recall $f(s) = s^2/(s^2 + m(1-s)^2)$; figure B.2 shows this curve with *viscosity ratio* $m = 1/2$. The well-known vanishing-viscosity solution to (B.1) is given by

$$s(x,t) = w(\eta)H[f'(s^-)vt - x] \quad \text{with} \quad x \geq 0,\ t > 0, \tag{B.2}$$

where $\eta = x/t$, $w(\eta)$ is the solution to $vf'(w(\eta)) = \eta$, and $s^-$ is defined below. The (water) saturation profile at a positive time is shown in figure B.1. Any monotone S-shaped function for $f(s)$ will lead to a qualitatively similar solution.

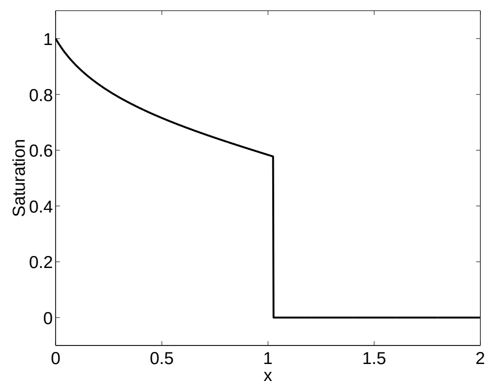


FIG. B.1. *Buckley–Leverett saturation profile at $t > 0$.*

We briefly review the solution of (B.2) within the context of §4.2. The rarefaction part of the solution is obtained from (4.6), here given by

$$-\eta \frac{ds}{d\eta} + v\, f'(s(\eta))\, \frac{ds}{d\eta} = 0, \tag{B.3}$$

so that $\eta = v\, f'(s(\eta))$. This simply states that $s(x,t)$ is constant along characteristics, and leads to the definition of $w(\eta)$ in (B.2). For $t > 0$, rarefaction is allowed as long as $f'(s(\eta))$ is increasing in $\eta$; otherwise a shock forms. The requirement $\nabla\lambda_k \cdot \mathbf{r}_k \neq 0$ for (4.7) reduces to $v\, f''(s) \neq 0$, a convexity condition that is violated at a point $s^*$ where $f''(s^*) = 0$. The rarefaction must connect to a shock at some value $s^- \geq s^*$. The condition (4.8), here given by

$$[s^+ - s^-]\dot{\xi}(t) = v\,[f(s^+) - f(s^-)], \tag{B.4}$$

gives us information about the shock $\xi$.

It is evident from the shape of $f'$ (figure B.2) that characteristics to the right of the shock must run into it, so that $s^+$ must be the initial value zero. Also, $\dot{\xi}$ must

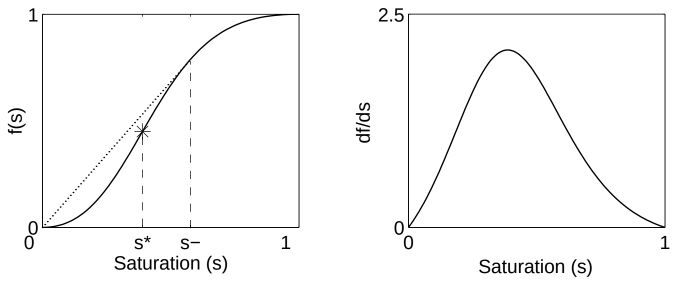


FIG. B.2. *The nonconvex fractional flow function and its first derivative.*

match the characteristic speed $\eta = v\, f'(s^-)$ just to its left. Combining these facts, we obtain $-s^- f'(s^-) = -f(s^-)$, which can be solved uniquely for $s^-$. It is the value of $s$ at which the secant of $f$ that passes through the origin is identical to the tangent of $f$. In our case, $s^- > s^*$. These arguments are analogous to the application of the Liu criterion in §4.3.

Physically, the profile in figure B.1 represents a smoothly varying mix of oil and water from the inflow boundary with a sharp transition to an oil-saturated zone.

## Appendix C. Algorithm for connecting $R_1$ to $S_2$ by a shock.

Define *tol* to be the error tolerance.

1. Choose $\mathbf{u}^- = \mathbf{u}^*$ on $R_1$. Define $\eta^*$ by $\mathbf{u}^* \equiv R_1(\eta^*)$.
2. Solve $\Phi(\mathbf{u}; \mathbf{u}^-) = 0$. Define $\mathbf{u}^+ = \mathbf{u}$ at the point of intersection with $S_2$.
3. Compute $\dot{\xi}_1 = [F_1(\mathbf{u}^+) - F_1(\mathbf{u}^-)]/[u_1^+ - u_1^-]$.
   (i) If $|\dot{\xi}_1 - \lambda_1(\mathbf{u}^-)| < tol$, then stop.
   (ii) Else if $\dot{\xi}_1 < \lambda_1(\mathbf{u}^-)$, then choose $\eta < \eta^*$.
   (iii) Else choose $\eta > \eta^*$.
4. Repeat at step 2.

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