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Probabilistic Forecast of Multiphase Transport Under Viscous and Buoyancy Forces in Heterogeneous Porous Media

Farzaneh Rajabi and Hamdi A. Tchelepi

Abstract We develop a probabilistic approach to map parametric uncertainty to output state uncertainty in first-order hyperbolic conservation laws. We analyze this problem for nonlinear immiscible two-phase transport in heterogeneous porous media in the presence of a stochastic velocity field. The uncertainty in the velocity field can arise from incomplete descriptions of either porosity field, injection flux, or both. This uncertainty leads to spatiotemporal uncertainty in the saturation field. Given information about spatial/temporal statistics of spatially correlated heterogeneity, we leverage the method of distributions to derive deterministic equations that govern the evolution of pointwise cumulative distribution functions (CDFs) of saturation for a vertical reservoir, while handling the manipulation of multiple shocks arising due to buoyancy forces. Unlike the Buckley-Leverett equation, the equation describing the fine-grained CDF is linear in space and time. Ensemble averaging of the fine-grained CDF results in the CDF of saturation. Thus, we give routes to circumventing the computational cost of Monte Carlo simulations (MCS), while obtaining a pointwise description of the saturation field. We conduct a set of numerical experiments for one-dimensional transport, and compare the obtained saturation CDFs, against those obtained using MCS as our reference solution, and the statistical moment equation method. This comparison demonstrates that the CDF equations remain accurate over a wide range of statistical properties, that is, standard deviation and correlation length of the underlying random fields, whereas the corresponding low-order statistical moment equations significantly deviate from the MCS results, except for very small values of standard deviation and correlation length.

1. Introduction

Long-term resource allocation, perspective planning, and risk mitigation of available energy resources rely on accurate modeling of the underlying physical phenomena. This includes simulating fluid flow and transport in complex geological formations, including applications like oil recovery, contaminant dispersion in aquifers, and carbon capture and sequestration. Deterministic modeling of flow and transport in such systems has been widely investigated for both single-phase and multiphase flow in numerous studies including Baqer and Chen (2022), Carrera et al. (2022), Fan et al. (2012), and Yousefzadeh (2020). Rigorous modeling of these systems primarily depends on sophisticated methodologies for uncertainty quantification of the system under study. Such an uncertainty is inherent to, and critical for, any physical modeling, essentially due to the incomplete knowledge of the state of the underlying system, noisy observations, and limitations in systematically recasting physical processes in a suitable mathematical framework. Furthermore, the available information about a particular geologic formation (e.g., from well logs and seismic data of an outcrop) is usually sparse and inaccurate compared to the size of the natural system and the complexity arising from multi-scale heterogeneity of the underlying system. Eventually, the uncertainty in flow predictions significantly influences oil recovery and contaminant transport predictions. Therefore, relying on a deterministic framework is no longer sufficient, calling for the development of probabilistic flow predictions. To this end, a stochastic framework is usually employed to describe the lack of knowledge about the spatial distribution of multiscale heterogeneous materials. Such a stochastic representation is the key building block for quantitative analysis of uncertainty propagation from system inputs to the output state variables of interest. Full probability distributions of the output states are then the essential means to quantify the uncertainty in the outputs. Within this stochastic framework, predicting the saturation fields means computing the joint probability distribution of the saturation, that results from the probabilistic distribution of spatial and/or temporal random inputs. Probabilistic analysis of flow and transport has been widely explored using various approaches. Earlier works of Gelhar (1986) and Rubin (2003) presented a comprehensive study for stochastic hydrology. Such stochastic frameworks quantify the associated uncertainty of the previously studied deterministic models.
Monte Carlo simulation (MCS) methods have been widely used to solve stochastic partial differential equations (PDEs) that describe flow and transport in heterogeneous media. Their popularity stems from their robustness and ease of implementation. Additionally, their convergence is guaranteed by the law of large numbers. However, MCS methods demand a substantial number of equi-probable realizations of inputs to achieve a reasonable accuracy. Hence, they suffer from a slow convergence rate, which is inversely proportional to the square root of the number of realizations. To accelerate convergence, various strategies have been introduced, among which Müller et al. (2013) employed Multilevel Monte Carlo (MC) to accelerate uncertainty quantification in a streamline-based two-phase flow model with a stochastic permeability field.

Stochastic spectral methods are another popular approach for estimating statistical moments in both single-phase and multiphase flow problems. These methods, studies by numerous authors (H. Li & Zhang, 2007; Müller et al., 2011; Shalimova & Sabelfeld, 2017; Xiú & Hesthaven, 2005; Zhang & Lu, 2004), work by truncating the Karhunen-Loève (KL) expansion or the polynomial chaos expansion of random processes, and are developed using either stochastic collocation methods (H. Li & Zhang, 2009), or stochastic Galerkin methods (Pettersson & Tchelepi, 2014). This category of methods has gained traction due to their faster predictive capabilities compared to MCS, as well as their capacity for rigorous convergence analysis (Ibrahima et al. (2018) and the references therein). However, in practical applications, they struggle with exponential complexity escalation concerning dimensionality and correlation scales, which is known as the curse of dimensionality. Moreover, the series’ convergence depends on the choice of correlation function (Exponential, Gaussian, etc.). Additionally, they often fall short in providing a complete statistical characterization of the problem, and require further sophistication for highly nonlinear problems, as proposed by Pettersson and Tchelepi (2014).

Statistical moment equations (SME), also known as low-order approximations (LOAs) derive deterministic equations for the leading statistical moments of the system states, by averaging stochastic PDEs. Even though this scheme provides the first two statistical moments (ensemble mean and variance) to forecast a system’s average response and its uncertainty, they fail to predict the probability of rare events (i.e., tails of the probability distribution), which is critical for risk assessment. Moreover, SME methods rely on perturbations, and hence, the moment estimates are accurate only for very small variances. Kitanidis (1988), Graham and McLaughlin (1989), Winter et al. (2003), L. Li and Tchelepi (2005), and Zhang and Winter (1999) employed this method for single-phase contaminant transport. In the context of multiphase flow problems, numerous studies were performed by Zhang et al. (2000) for the Lagrangian treatment of moment equations subject to a stochastic permeability field, and also for the Eulerian moment equations by Jarman and Russell (2003), and for the forward and inverse modeling of immiscible two-phase flow by Likanapaisal et al. (2012), in which the equations governing the statistical moments of the quantities of interest are derived and solved directly.

This deficiency in predictive capabilities of SME methods can be tackled by using the probabilistic method of distributions, that is, probability density function (PDF) or cumulative density function (CDF) methods. First introduced in the turbulence flow literature by Pope (1985), the PDF/CDF methods provide a pointwise marginal probabilistic distribution by deriving deterministic equations for PDFs or CDFs of the system states. While the formulation of boundary conditions for PDF methods is not unique, CDF schemes tend to have uniquely formulated boundary conditions in a straightforward and unambiguous manner. Also, PDF methods may occasionally require problem-specific closures, not always conveniently attainable. Meyer and Tchelepi (2010), Meyer et al. (2010), and Meyer et al. (2013) have utilized the PDF method for a particle-based single-phase transport of a stochastic total-velocity field using a Markovian approximation. Furthermore, Yang et al. (2019) have presented a comparison between the CDF method, SME, and MCS for steady-state single-phase flow, demonstrating robustness and computational advantage of the CDF method over both MCS and SME.

Stochastic treatment of immiscible multiphase transport, that is, the Buckley-Leverett (BL) model in highly heterogeneous media poses additional challenges compared to their single-phase counterparts. This originates from nonlinearity of the transport equation and coupling of the total-velocity, pressure and saturation fields. The nonlinearity stems from the fact that the uncertain velocity field depends on the system state itself. Earlier studies focused on streamline-based strategies for solving flow (pressure and velocity), and transport (saturation) problems, that is, the Buckley-Leverett equation, and provided the statistics for the travel-time metric. Several studies in this context were conducted by Ibrahima et al. (2015) for single-point probability distribution of one-dimensional highly-heterogeneous porous media, in which the CDF obtained from the streamline-based simulation approach was found to be more efficient than MC simulations of the nonlinear transport equation. Moreover, Ibrahima
et al. (2018) investigated single-point multi-dimensional (applicable to two- or three-dimensional) heterogeneous formations by using the frozen (i.e., time-independent) streamline distribution method (FROST). Streamline-based studies provide a robust Lagrangian framework for tracing fluid particles from injection to production wells in multiphase flow problems. However, more intricate cases involving buoyancy forces require an alternative approach. These cases encompass the interaction of multiple shocks and their reflection from boundaries. To effectively handle such scenarios, employing a front-tracking mass-conservative Eulerian upwinding scheme, such as the Godunov method, is required (Harten et al., 1983). This approach accurately captures the complex interactions of multiple waves and discontinuities, offering a valuable solution for accurate modeling of these challenging problems. Another study by Ibrahima and Tchelepi (2017) extended the single-point CDF approach to multi-point distribution of saturation in two-phase transport, where they have included the covariance function of saturation in order to build appropriate confidence intervals. Fuks et al. (2019) extended the argument of Ibrahima et al. (2015) to estimate the statistics of fluid saturations in channelized porous systems by using the frozen streamline assumption of the FROST scheme. In the context of multiphase flow problems, Wang et al. (2013) proposed a framework to estimate single-point CDFs of saturation for the one-dimensional Buckley-Leverett problem, in which the time-dependent total flux is assumed to be stochastic, leading to a stochastic total velocity field which is characterized by a known distribution. They derive a general deterministic equation for the single-point CDFs of saturation for a horizontal reservoir, in which gravity segregation plays no role.

Numerous studies (Brenier & Jaffré, 1991; Kwok & Tchelepi, 2008; B. Li & Tchelepi, 2014, 2015; B. Li et al., 2013; Lie, 2019; Tchelepi, 1994; Zaleski & Panfilov, 2017) have investigated the deterministic behavior of buoyancy forces interacting with viscous and capillary forces in multiphase hyperbolic transport models. Moreover, while uncertainty assessment for hyperbolic conservation laws (kinematic wave models) has been explored in several studies (Cheng et al., 2019; LeVeque, 2002; Zaleski & Panfilov, 2017), no study has been conducted on evaluating the single-point distribution of saturation for stochastic nonlinear first-order hyperbolic conservation laws in two-phase flow models, in which buoyancy forces have been taken into account. Our study proposes an efficient semi-analytical distribution method for estimating the single-point CDF of saturation for the BL model in one-dimension, for a vertical reservoir with gravitational forces considered. More specifically, we investigate the horizontal, updip and downdip flooding scenarios as well as pure gravity segregation in an inverted gravity column. Unlike the BL equation, the resulting equation for the CDF is linear in space/time, and is solved semi-analytically for one-dimensional problems and numerically for higher dimensions. This framework results in a pointwise probabilistic description of the saturation field for different physical setups, offering a computationally efficient alternative to exhaustive MC simulations.

In Section 2, we delve into the governing equations of the Buckley-Leverett problem, elucidating disparities in the flux functions between horizontal and gravitational case studies. Section 3 outlines the CDF method, followed by the derivation of deterministic equations for the single-point CDF of saturation incorporating gravitational forces, subject to a random porosity field and/or random injection flux. In Section 4, we illustrate numerical aspects of uncertainty quantification for nonlinear hyperbolic Buckley-Leverett (BL) equation with three different approaches, that is, MCS, SME, and the CDF method. We leverage the mass-conservative finite volume Godunov scheme to perform MC simulations for the Riemann problem of the BL equation as our reference solution, followed by comparing its solution for several test cases against those of our CDF method and the low-order SME approximations. A more comprehensive analysis of LOA for different random quantities is offered in Section 5. We conclude this study by analyzing the accuracy, convergence and sensitivity of our proposed method in Sections 6 and 7, followed by the conclusion in Section 8.

2. Problem Formulation

We consider nonlinear, incompressible, two-phase (Darcy) flow in a heterogeneous reservoir with an intrinsic permeability field \( k \), and a spatially-varying porosity field \( \phi(x) \) in the one-dimensional domain, where there are two immiscible phases; water and oil. The key underlying physical mechanisms are viscous and gravitational forces, whereas capillarity, chemical reactions, diffusion, and changes of state are neglected. We are primarily interested in estimating saturation fields while quantifying the uncertainty associated with their description for horizontal domains as well as vertical reservoirs in which gravity segregation plays a major role throughout the displacement process.
The inherent uncertainty in the response parameters arises from various sources of uncertainty in the input parameters of the reservoir. These input specifications include initial saturations of water and oil \( (S_w, S_o) \), boundary conditions for water \( (S_w(x=0, t) \) at the inlet of the domain), parameters representing the fluid properties, such as water and oil viscosities \( (\mu_w, \mu_o) \), parameters describing rock properties, such as porosity and permeability \( (\phi(x) \) and \( (k(x)) \), parameters outlining the fluid-rock interactions, such as relative permeabilities \( (k_{rw}(S_w), k_{ro}(S_o)) \), as well as the injection and production pressures of water \( (P_{in} \) and \( P_{prod}) \).

An ideal prediction scenario calls for the complete knowledge of all the aforementioned parameters. However, data sparsity and heterogeneity of the input definitions render such a framework unattainable. The primary justification to consider the inputs as stochastic variables is having limited measurements which are only available at well locations, for the static properties (porosity, permeability) as well as dynamic properties (saturation, injection/production rates) of the reservoir. Since we are considering a one-dimensional domain, we exclude the consideration of a stochastic permeability field. Instead, we focus on the uncertainty in the porosity field \( \phi(x) \) and the total Darcy flux \( q(t) \), while assuming all the remaining parameters to be deterministic. More precisely, we describe these random parameters using a prescribed PDF, that is, by assigning a specific probabilistic description \( p_x(\phi) \) and \( p_k(Q) \) to them, characterized by their known mean \( (\mu) \), standard deviation \( (\sigma^2) \), and correlation structure \( (C_r) \). Then, we propagate the uncertainty from inputs to output quantities of interest, essentially by solving a coupled system of nonlinear transport equations for saturation which satisfies mass conservation, along with the Darcy equation for pressure field. This standard framework enables us to identify a probabilistic spatio-temporal description for the water saturation.

### 2.1. Governing Equations

The nonlinear hyperbolic conservation law with a non-convex flux is conventionally studied by employing the Buckley-Leverett (BL) equation, which results from combining mass balance for each phase \( \alpha = w, o \) with Darcy’s law (Buckley & Leverett, 1942). For a horizontal reservoir, this equation reads (Appendix A):

\[
\frac{\partial S_w}{\partial t} + v_T(x, t)f_w(S_w)\nabla S_w = 0, \quad \text{where} \quad v_T = q(t)\phi(x)
\]

\[
S_w(x=0, t) = S_w^i, \quad S_o(x, t) = S_o, \quad x \in \bar{\Omega}, t > 0,
\]

\[
S_w(x, t=0) = S_{w, i} = \frac{k_{rw}}{k_{rw} + mk_{ro}}(1 - N_g k_{ro} \sin \theta)
\]

which is indeed in the form of an advection equation with velocity \( v_T(x, t) \equiv \frac{q(t)}{\phi(x)} f_w(S_w) \). In this equation, \( v_T(x, t) \) denotes the interstitial velocity (total seepage velocity field), and \( q(t) \) is the total volumetric flow rate, obtained by multiplying the total Darcy velocity by the area \( A \) (In this study, \( A \) is assumed to be 1.). Furthermore, \( f_w(S_w) \) denotes the fractional flow of water, which is a continuous, smooth and hence differentiable function, defined as follows:

\[
f_w(S_w, \theta) = \frac{k_{rw}}{k_{rw} + mk_{ro}}(1 - N_g k_{ro} \sin \theta)
\]

where \( m = \frac{\mu_o}{\mu_w} \) is the viscosity ratio, \( \theta \) denotes the dip angle of an inclined reservoir, and \( N_g \) is the dimensionless gravity number, defined as the ratio of buoyancy to viscous forces:

\[
N_g = \frac{k g (\rho_o - \rho_w)}{\mu_w \omega_T}
\]

Furthermore, \( k_{rw}(\alpha = o, w) \) denote relative permeabilities of each phase. There are several empirical models for defining the relative permeabilities as a function of water saturation. Brooks and Corey (1964) and Van Genuchten (1980) are the most commonly employed empirical models. We opt to employ the quadratic Brooks-Corey model to define relative permeabilities given by the following expressions:

\[
k_{rw}(S_w) = \left( \frac{S_w - S_{wi}}{S_B - S_{wi}} \right)^2, \quad k_{ro}(S_o) = \left( \frac{S_o - S_{wi}}{S_B - S_{wi}} \right)^2
\]

In Equation 1, the initial water saturation in the domain \( \Omega \) is denoted by \( S_{w,i} \). In other words, the reservoir is assumed to be initially oil-saturated with a small irreducible water saturation \( S_{wi} \). \( S_B \) is water saturation at the
injection boundary $\Gamma_r$ that is, $x = 0$, where water is being injected. $S_w$ is the irreducible oil saturation. $\Gamma_o$ is the boundary along which the flow outlet happens. Although initial/boundary conditions may be in general random variables, we assume they are both deterministic constants. Also, in order to guarantee self-similarity in solutions of saturation, we impose $S_w$ and $S_B$ as uniform in space and time-independent quantities. For the test cases with gravitational force included, the initial condition is non-uniform. Moreover, the following Dirichlet boundary conditions are considered for the pressure field (pressure control):

$$P(x) = p_{vo}, \quad x \in \Gamma_r, \quad P(x) = p_{pat}, \quad x \in \Gamma_o$$

(5)

In the pure gravity segregation scenario, we consider a vertical column in a heterogeneous domain with sealing top and bottom boundaries, so $q_T = 0$. We assume the heavier (more dense) fluid on the top and the lighter fluid beneath. This setup gives rise to an unstable situation which needs to reach a vertical equilibrium. Therefore, even though $u_T = 0$, we have $u_r \neq 0$, $u_o \neq 0$, where the continuity condition results in $u_o + u_r = \text{constant}$. Assuming boundary conditions $u_o = u_r = 0$ at the top and bottom of the domain, we conclude the constant is zero, and hence $u_r = -u_o$. Consequently, $u_p = 0$ entails a revised definition for $f_w$, as we can no longer use the conventional definition in Equation 2. The fractional flow for this case is defined as:

$$G(S_w) = \frac{k_{rw}}{1 + (k_{rw} \mu_o/k_{rw} \mu_w)}$$

(6)

Subsequently, the transport equation is recast as:

$$\frac{\partial S_w}{\partial t} + \frac{u_r}{\phi(z)} G_w'(S_w) \cdot \nabla S_w = 0$$

$$S_w(z = 0, t) = S_B = 1 - S_{wi}, \quad z \in \Gamma, t > 0,$$

$$S_w(z, t = 0) = 1 - S_{wi}, \quad z \in \Omega^- \equiv [0, z_d]$$

$$S_w(z, t = 0) = S_{wi}, \quad z \in \Omega^+ \equiv [z_d, L]$$

(7)

A hyperbolic conservation law with a piecewise constant initial condition of the form:

$$S(z, t = 0) = S_0(z) = \begin{cases} S_L & z \leq z_d \\ S_R & z > z_d \end{cases}$$

(8)

forms a Riemann problem, where $S_L$ and $S_R$ denote the left and right values of the initial condition, separated at a discontinuity location denoted by $z_o$. While in general, $S_L$ and $S_R$ can be random, we assume they are deterministic constants. As the flux function changes its convexity throughout the saturation domain, the solution of this Riemann problem can be comprised of shocks and rarefaction zones, depending on whether the flux function is convex or concave over that specific interval. The exact analytical solution to Equation 1 subject to the given boundary/initial conditions, in one-dimensional domain of $[a,b]$, and a final simulation time $T$, for a given realization of the total velocity $v_f(x, t)$, can be expressed as following Orr (2007):

$$S_w(x, t; v) = \begin{cases} S_B, & x < X_1 \\ S_t = (f_w' \phi)^{-1} \left[ x \left( \frac{\partial^2 S_t}{\partial x^2} \right)^{-1} \right], & X_1 \leq x < X_2 \\ S_{wi} & x \geq X_2 \end{cases}$$

(9)

where $X_1 = \alpha$ and $X_2 = x_r(t; v)$ for the no-gravity case. Whereas the solution for downsip flooding and gravity column before reflection of the waves takes into account the presence of two shocks, resulting in the same solution above, however, $X_1 = x_f_r(t; v)$ and $X_2 = x_f_l(t; v)$, where $x_f_i(t; v)$ for $i = 1, 2$ describes the front location at time $t$ for the given realization of total velocity. This quantity can be found by satisfying the entropy constraint through the Rankine-Hugoniot condition at the location of discontinuities (shocks):

$$\frac{dx_{f_i}}{dt} = \frac{q(t) f_w (S^*_t) - f_w(S_{wi})}{\phi(x)} \left( S^*_t - S_{wi} \right)$$

(10)
where the critical saturation level, denoted as \( S^*_i \), is determined by enforcing the continuity condition on the shock speed:

\[
\frac{f_w(S^*_i) - f_w(S_{wi})}{S^*_i - S_{wi}} = f_w'(S^*_i)
\]

(11)

It is noteworthy that \( S^*_i \) is independent of the total velocity and hence, it is deterministic at a given time. For the special case of horizontal reservoir domain (with fractional flow \( f_w = \frac{k_{rw}}{k_{ro} + k_{rw}} \) supplemented by Brooks-Corey relative permeabilities), \( S^*_i \) has an analytical expression (Equation 4.7 in Ibrahima and Tchelepi (2017)). Nevertheless, we resort to a general numerical root finding scheme which handles \( N_s \neq 0 \) cases as well.

### 2.2. Fractional Flow

Predictions of two-phase flow entail solving the first-order nonlinear hyperbolic Buckley-Leverett equation with a non-convex flux (the flux function changes its convexity within the given saturation interval). The evolution of the saturation field is generally described in terms of nonlinear kinematic waves, where different complex wave propagation scenarios happen, depending on the initial/boundary conditions as well as behavior of the flux function, that is, whether the flux function includes gravity or not, and if it does, how the convexity of flux function changes throughout the domain. These scenarios include formation of shocks and rarefaction zones as well as reflection of shocks from endpoints of the domain. Illustrating behavior of the flux function necessitates full specification of the dip angle and relative permeabilities. According to Equation 2, the fractional flow is a function of both saturation and the dip angle, giving rise to three distinct scenarios based on the inclination angle \( \theta \):

- **When** \( N_s \sin \theta = 0 \), Equation 2 simplifies to that of a horizontal reservoir, signifying the absence of gravity and making viscous forces the sole driving mechanism.
- **For** \( N_s \sin \theta > 0 \), updip flooding occurs, where gravity hinders the water’s advance, resulting in a reduced front velocity. Notably, \( \sin \theta > 0 \) can yield a fractional flow smaller than 0. Assuming that water is heavier (i.e., more dense) than oil, \( f_w < 0 \) signifies the counter-current flow of water (the heavier phase) moving updip, while oil (the lighter phase) phase moves updip. In the range \( 0 < f_w < 1 \), water and oil co-currently flow updip.
- **For** \( N_s \sin \theta < 0 \), a downdip flooding scenario emerges, with gravity intensifying water flow and hence accelerating the saturation front’s movement. In this situation, oil experiences counter-current flow, moving updip, while water flows downdip in the inclined reservoir. \( \sin \theta < 0 \) leads to \( f_w > 1 \). Conversely, in the \( 0 < f_w < 1 \) range, both phases move downdip co-currently.

The flux functions corresponding to these scenarios are schematically represented in Figure 1. Horizontal case \((N_s = 0)\) with an S-shaped curve is characterized by a shock and a trailing rarefaction zone where viscous forces are the only driving mechanism, whereas the vertical updip injection \((N_s = 10)\) is characterized by a shock and a rarefaction zone, and vertical downdip injection case \((N_s = −10)\) is characterized by two shocks and a rarefaction zone in between. The two former cases represent the combined effect of viscous and buoyancy forces. The case in sub-figure (d) represents the pure gravity segregation in an inverted gravity column and is physically similar to the downdip scenario, except that it has sealed boundaries at the top and bottom. That is, in the downdip flooding scenario, we inject at one boundary, and recover from the other boundary. On the other hand, in the pure gravity segregation case, we assume that buoyancy governs the entire physics without the assistance of injection or viscous forces.

To this end, we consider a gravity column in a heterogeneous domain, confined by a sealing medium at the top and bottom. We define an initial condition with a heavy fluid on top of a lighter fluid, described by setting \( S_{zL} = 1 \) in the top half of the domain and \( S_{zK} = 0 \) in the bottom half of the domain. The fluids are separated by a sharp interface, and initially the interface is at \( Z = 1 \). Then, the two fluids start segregating, where the heavier fluid would like to move downward (positive \( z \) direction) and reside below the lighter one, and hence the lighter fluid moves upward (negative \( z \) direction). While the shock regions are representative of a single-phase fluid, the rarefaction area is indeed two-phase. Therefore, the outer envelope shows the two waves before hitting the boundaries for the first time. These waves in the downdip displacement and gravity column cases move in the opposite directions and will be eventually reflected from each boundary, schematically shown by the inner envelope. Note that \( m \neq 1 \), and the corresponding flux function is asymmetric, and hence, the two waves move asynchronously, that is, one may hit its boundary earlier than the other, depending on \( m \). Once reflected from both boundaries, the
waves follow a very small rarefaction region. Afterwards, at $A_AHH$ and $A_AHH$, two shocks form again, start moving towards each other and meet at a point, denoted by $z_j$. Subsequently, they reach equilibrium at $t_{eq}$, where the initial condition has been completely flipped.

### 2.3. Nondimensionalization

We will investigate how uncertainty in the inputs affects the output saturation field, first by assuming that $\phi(x)$ is random and $q$ is a deterministic constant, second by assuming that $q(t)$ is random and $\phi$ is a deterministic constant, and third by assuming both are stochastic fields. For the case in which $q(t)$ is random, characterized by the given mean $\mu_q$ and correlation length $\tau_q$, we nondimensionalize the transport Equation 1 for each realization of the velocity field by defining:

$$x_D = \frac{x}{L}, \quad t_D = \frac{1}{L} \int_0^t q(t') dt'$$

For the cases in which $q$ is a deterministic constant, we use the dimensionless quantities below to nondimensionalize Equation 1:

$$x_D = \frac{x}{L}, \quad t_D = \frac{q t}{L}$$

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**Figure 1.** Illustration of the continuous (analytical) fractional flow curves for the four case studies of our problem: (a) horizontal displacement, (b) upslope background drift, (c) downslope background drift and (d) pure gravity segregation. The dashed curves correspond to the flux function $f_w(S_w)$. For cases (b) and (c), $f_w(S_w)$ accounts for a combination of gravitational forces and viscous background drift. The blue lines represent concave envelopes, indicating injection at the left edge of the domain. Conversely, the red lines denote the convex envelopes, indicating drainage at the right edge. In case (d), the inner envelope indicates reflection of waves from the boundaries. All cases adopted the Brooks-Corey relative permeabilities, and have a viscosity ratio of $m = 0.5$. 

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These definitions lead to the dimensionless form of Equation 1 in the one-dimensional domain Ω:

$$\phi(x) \frac{\partial S_w}{\partial t_B} + \frac{\partial f(S_w)}{\partial x_D} = 0$$

To nondimensionalize the transport Equation 7 for the pure gravity segregation case, where no injection flux is present, our focus will be solely on examining the impact of the random porosity field on water saturation. Therefore, we introduce the following dimensionless time and distance parameters:

$$t_D = t \frac{g(\rho_o - \rho_w)k}{\mu_w H} = \frac{t}{\tau}, \quad z_D = \frac{z}{H}$$

where $H$ is the total length of the vertical domain and $\tau = \mu_w H/g(\rho_o - \rho_w)k$ is the characteristic time scale for gravity segregation. That is, if $\tau = 1$, a fluid parcel has enough time to travel across the entire length of $H$. These definitions lead to the dimensionless form of Equation 7 as follows:

$$\phi(z) \frac{\partial S_w}{\partial t_D} + \frac{\partial G(S_w)}{\partial z_D} = 0$$

3. Single-Point CDF Equation for Saturation

In order to provide a pointwise CDF of water saturation, we solve a deterministic equation that governs the space-time evolution of the CDF of water saturation $F_s(S_w; x, t)$, while incorporating the influence of gravitational forces. This approach overcomes the limitations of solving the nonlinear hyperbolic Equations 1 and 7, by introducing a random raw (fine-grained) CDF function of water saturation. This fine-grained (raw) CDF, which is primarily done by adding a kinetic defect term for numerous MC realizations of random variables, followed by the derivation of the CDF for the output saturation.

For continuous solutions of Equations 1 and 7, the linear hyperbolic equation for the random fine-grained CDF reads (details outlined in Appendix B):

$$\frac{\partial \Pi}{\partial t} + v_i(\theta, x, t) \cdot \nabla \Pi = 0 \quad x \in \Omega, t > 0$$

$$\Pi(\theta, S_w; x, t = 0) = H(\theta - S_{w0})$$

where the boundary condition corresponds to the injection of water at the inlet $x = 0$. As mentioned before, Equation 19 holds only for the continuous solutions of the fine-grained CDF, in which we are excluding the treatment of shocks (discontinuities). A general form of Equation 19 consists of imposing non-smooth solutions to fulfill entropy conditions at the location of discontinuities, allowing for a physically meaningful solution. This is primarily done by adding a kinetic defect term $M(\theta, x, t)$ to Equation 19, making it:

$$\frac{\partial \Pi}{\partial t} + v_i(\theta, x, t) \cdot \nabla \Pi = M(\theta, x, t)$$

Therefore, we determine the spatiotemporal evolution of $F_s(\theta; x, t)$, by initially solving a linear equation for $\Pi$, and then considering only its ensemble mean. This methodology offers a more straightforward route compared to the initial process of numerically solving the nonlinear Equations 1 and 7 for numerous MC realizations of random variables.
which essentially results in a valid solution for the entire domain of saturation. While higher-dimensional problems require solving Equation 20 in lieu of Equation 19, their one-dimensional counterparts avoid the additional complexities that arise from wave interactions in higher dimensions. Consequently, the one-dimensional problem could be studied by employing Equation 19 for the distinct smooth segments of the domain. To this end, for horizontal displacement and updip flooding, we divide the solution of Equation 19 into two sub-regions, similarly to Wang et al. (2013):

\[
\Pi(\theta; x, t) = \begin{cases} 
\Pi_a = H(\theta - S_w), & S_w < \theta < S^*, \quad x_f(t; v) < x < b \\
\Pi_b = H(\theta - S_v), & S^* < \theta < 1 - S_v, \quad a < x < x_f(t; v)
\end{cases}
\] (21)

For the downdip flooding case and for the pure segregation scenario before the fastest-moving wave reaches its boundary, we deal with three sub-regions. That is, for \(0 < t < t_{ref1},

\[
\Pi(\theta; x, t) = \begin{cases} 
\Pi_a = H(\theta - S_w), & S_w < \theta < S^*_w, \quad x_{fa}(t; v) < x < b \\
\Pi_b = H(\theta - S_v), & S^*_w < \theta < S^*_l, \quad x_{fa}(t; v) < x < x_{fa}(t; v) \\
\Pi_c = H(S_B - \theta), & S^*_l < \theta < 1 - S_v, \quad a < x < x_{fa}(t; v)
\end{cases}
\] (22)

Note that there are no reflections of waves from boundaries for the downdip case. Also, it should be noted that \(\Pi_a, \Pi_b, \Pi_c, \Pi_e, \Pi_d, \Pi_g, \Pi_i, \Pi_h, \Pi_j, \Pi_k\) are independent of \(x\) and \(t\). In the case of pure gravity segregation, once the waves bounce off the boundaries, they give rise to three distinct rarefaction fans, accompanied by two shocks situated in between, where the shocks move towards each other. As depicted in Figure 2, the rarefaction region in the middle is indeed the continuation of the characteristics in the rarefaction fan of the region \(\Pi_b\) in Equation 22, up to the time \(t_f\). Eventually, when the two shocks meet at time \(t_j\), they form one shock along with two rarefaction zones. Therefore, at \(t = t_j\), the middle rarefaction area has totally disappeared and we have \(x_{fa}(t; v) = x_{fa}(t; v) = x_{eq}\). For the inverted gravity column case, after the slowest-moving wave has reflected from its boundary, that is, for \(t_{ref2} < t < t_j\), we deal with the following sub-regions:

\[
\Pi(\theta; x, t) = \begin{cases} 
\Pi_a = H(\theta - S_{w1}), & S_{w1} < \theta < S^*_l, \quad a < x < x_{fa}(t; v) \\
\Pi_b = H(\theta - S_v)H(t_f - t) + 0 \cdot H(t - t_j), & S^*_w < \theta < S^*_l, \quad x_{fa}(t; v) < x < x_{fa}(t; v) \\
\Pi_c = H(\theta - S_{w2}), & S^*_l < \theta < 1 - S_v, \quad x_{fa}(t; v) < x < b
\end{cases}
\] (23)
Moreover, it is worth noting that, similarly to the previous literature (Ibrahima & Tchelepi, 2017; Wang et al., 2013), we prefer employing the CDF framework rather than working with the PDF equations. This preference arises from straightforward formulation of boundary conditions in the CDF methodology, that is, \( F_2(\theta = S_{wi}; x, t) = 0 \) and \( F_2(\theta = 1 - S_{wi}; x, t) = 1 \). Whereas, the boundary conditions can not be uniquely defined for the PDF scheme. Furthermore, adopting the CDF approach eliminates the need to address closure approximations inherent in the PDF scheme.

The method of characteristics can be utilized to form an analytical solution for the one-dimensional linear hyperbolic Equation 19, specifically within the continuous rarefaction zone where no discontinuity is present.

While Wang et al. (2013), and Ibrahima and Tchelepi (2017) have explored the analytical solution of the CDF of saturation for a horizontal reservoir, our study delves into the more comprehensive scenario of vertical reservoirs involving the manipulation of multiple shocks, as emerged by buoyancy forces. The fine-grained CDF solution for the horizontal reservoirs reads (Wang et al., 2013):

\[
\Pi_b(\theta; x, t) = H(\theta - S_{wi})H(x - C) + H(\theta - 1 + S_{wi})H(C - x)
\] (24)

In order to define a family of characteristics \( x = x(t; x_o) \) along which the original hyperbolic PDE becomes an ODE of the form \( \frac{dx}{dt} = v(\theta, x(t), t) \), subject to \( x(t = 0) = x_o \), where \( x_o \) specifies where the characteristic line has originated from. Thus \( x = \int_0^t v(\theta, x(t'), t') dt' + x_o \). For the aforementioned setting of our problem, that is, the initial and boundary conditions of the gravity column, the characteristic solution is depicted in Figure 2. The non-unity viscosity ratio causes an asymmetry and asynchronism in the movement of two waves. To this end, we leverage the method of characteristics to construct the fine-grained CDF solution for the inverted gravity column, similarly to Equation 24. We build this solution in four distinct regions, that is, for the right-moving branch before and after being reflected from the right boundary (I and II, respectively), and similarly, for the left-moving branch before and after being reflected from the left boundary (III and IV, respectively) as outlined in Equation 25.

To construct the solution for \( \Pi_b \), we start with the right-moving wave, for which the saturation ranges from \( S_{wi} \) to the discontinuity point, denoted by saturation \( S_p \). As Figure 2 displays, before the right-moving wave reaches its boundary \( t < t_{ref2} \), all characteristics emanate from the \( z \) axis where \( t = 0 \). Therefore, the initial condition is used to build the solution (region I). After the right-moving wave bounces off the right boundary (region II), \( t_{ref2} < t < t_j \), the characteristics develop from the \( t \) axis at the right boundary (\( z = L \)), and continue up to \( t_j \) and the location \( z_{ref} \) where this left-moving branch meets the other right-moving branch coming toward it. To this end, the saturation at the right boundary \( S_p \) is used to construct the solution. For the left-moving wave, before it hits the left boundary \( t < t_{ref1} \), the saturation ranges from \( S_p \) to \( S_{wi} \). Therefore, the solution in region III is constructed by leveraging the saturation of the discontinuity point \( (S_p) \). We follow a similar logic for the left-moving wave after it hits the left boundary. At \( t = t_{ref1} \), the left-moving wave gets reflected from the left boundary, causing the characteristics to originate from the \( t \) axis where \( z = 0 \) (region IV), hence, we leverage \( S_{wi} \) to build the solution. In summary, the solution for \( \Pi_b \) comprises two parts: \( \Pi_{bR} \) and \( \Pi_{bL} \), where they represent the development of characteristics in the right and left branches, respectively, as outlined below:

\[
\Pi_b = \begin{cases}
\Pi_{bR} = & H(\theta - S_{wi})H(x - C) + H(\theta - S_p)H(C - x), \quad 0 < t < t_{ref2} \quad (I) \\
& H(\theta - S_p)H(x - C) + H(\theta - S_{wi}^*)H(C - x), \quad t_{ref2} < t < t_j \quad (II) \\
\Pi_{bL} = & H(\theta - S_p)H(x - C) + H(\theta - S_{wi})H(C - x), \quad 0 < t < t_{ref1} \quad (III) \\
& H(\theta - S_{wi})H(x - C) + H(\theta - S_{wi}^*)H(C - x), \quad t_{ref1} < t < t_j \quad (IV)
\end{cases}
\] (25)

where \( C(\theta; x, t) \) is defined as follows:

\[
C(\theta; x, t) = \int_0^t v(\theta, x(t'), t') dt' = \frac{1}{\phi(x)} \frac{\partial f(\theta)}{\partial \theta} \int_0^t q(t') dt' + \frac{\partial f(\theta)}{\partial \theta} \int_0^t v(x, t') dt'
\] (26)
Also, the following initial and boundary conditions are utilized for building the solution above:

\[ \Pi(\theta, x, t = 0) = H(\theta - S_{wi}), \]  

\[ \Pi(\theta, x = 0, t) = H(\theta - S_B) = H(\theta - 1 + S_w), \]  

\[ \Pi(\theta, x = x_d, t) = H(\theta - S_D) \]  

It should be noted that the fine-grained CDF solution for the downdip flooding scenario is defined only for regions I and III in Equation 25, as having sealed boundaries implies the absence of reflections from boundaries. We will present the general formulation of the CDF of water saturation, with uncertainty in both porosity field and injection flux encapsulated in:

\[ U(x, t) = \int_0^t \frac{q(t')}{\phi(x)} \, dt' \]  

For the cases with one shock, that is, a horizontal reservoir and a vertical reservoir with updip flooding, the CDF of saturation is then formulated as below (Wang et al., 2013):

\[ F_1(\theta; x, t) = \begin{cases} 
\int_0^\theta \Pi_u H(x - x_f) P_v(u) du, 0 \leq \theta < S^* \\
\int_0^\theta \Pi_u H(x - x_f) P_v(u) du + \Pi_t H(x_f - x) P_v(u) du, 0 \leq \theta \leq 1 - S_w \end{cases} \]  

We introduce \( F_{U,(x,t)} \), the CDF of the random input velocity field \( U(x, t) \), and employ the notation \( a \vee b := \max(a, b) \) and \( a \wedge b := \min(a, b) \). In order to directly map the uncertainty from inputs to the output saturation field, we adopt a similar approach to Ibrahima and Tchelepi (2017), and introduce the following relations for the CDF of water saturation (derivations outlined in Appendix C). For the horizontal and updip flooding scenarios, we expand Equation 31 as explained in Equation C1, and express the CDF of saturation corresponding to \( S_w \leq \theta < S^* \) as follows:

\[ F_{\omega}(\theta; x, t) = H(\theta - S_w)F_U \left( \frac{x}{f'(S^*)} \right) \]  

As the derivations are presented in Equation C2, for the saturation interval \( S^* \leq \theta \leq 1 - S_w \), we define the CDF as follows:

\[ F_{\omega}(\theta; x, t) = F_{\omega}(\theta; x, t) + H(\theta - S_w) \left( F_U \left( \frac{x}{f'(\theta)} \right) - F_U \left( \frac{x}{f'(S^*)} \right) \right) + H(\theta - S_B) \left( 1 - F_U \left( \frac{x}{f'(\theta)} \vee \frac{x}{f'(S^*)} \right) \right) \]  

Note that CDFs are cumulative quantities. Therefore, for each wave, it is necessary to aggregate the saturation CDFs from all the preceding times. Following a similar logic to Equation 31, we formulate the CDF equations for both the downdip scenario and the inverted gravity column case prior to the waves’ reflection from boundaries, as outlined below:

\[ F_1(\theta; x, t) = \begin{cases} 
\int_0^\theta \Pi_u H(x - x_f) P_v(u) du, 0 \leq \theta < S^*_R \\
\int_0^\theta \Pi_u H(x - x_f) + \Pi_k H(x_f - x) \right) P_v(u) du, S^*_R \leq \theta \leq S_D \\
\int_0^\theta \Pi_k H(x - x_f) \right) P_v(u) du, S_D \leq \theta \leq S^*_L \\
\int_0^\theta \Pi_k H(x - x_f) + \Pi_l H(x_f - x) \right) P_v(u) du, S^*_L \leq \theta \leq 1 - S_w \end{cases} \]  

As outlined in Appendix C, this equation expands as follows: For \( x > x_d, S_w < \theta < S^*_R \), following derivations in Equation C6, we establish:

\[ F_{\omega}(\theta; x, t) = H(\theta - S_w)F_U \left( \frac{x}{f'(S^*_R)} \right) \]
For \( x > x_{ir}^{*}, S_R^{*} < \theta < S_D \), as explained in Equation C7, we introduce:

\[
F_{s_k} (\theta; x, t) = F_{s_1} (\theta; x, t) + H(\theta - S_{wi}) \left( F_U \left( \frac{x}{f'(\theta)} \right) - F_U \left( \frac{x}{f'(S_R^{*})} \right) \right) \\
+ H(\theta - S_D) \left( 1 - F_U \left( \frac{x}{f'(\theta)} \vee \frac{x}{f'(S_R^{*})} \right) \right)
\]  

(36)

Furthermore, for \( x < x_{ir}^{*}, S_D < \theta < S_R^{*} \), as outlined in Equation C8, we present:

\[
F_{s_k} (\theta; x, t) = H(\theta - S_B) \left( F_U \left( \frac{x}{f'(S_R^{*})} \right) - F_U \left( \frac{x}{f'(\theta)} \right) \right) \\
+ H(\theta - S_D) \left( F_U \left( \frac{x}{f'(\theta)} \wedge \frac{x}{f'(S_R^{*})} \right) \right)
\]  

(37)

Eventually, for \( x < x_{ir}^{*}, S_R^{*} < \theta < S_B \), we formulate the CDF as detailed in Equation C9, leading to:

\[
F_{s_k} (\theta; x, t) = F_{s_1} (\theta; x, t) + H(S_B - \theta) \left( 1 - F_U \left( \frac{x}{f'(S_R^{*})} \right) \right)
\]  

(38)

For the pure gravity segregation scenario after the reflection of waves, the CDF relation is defined as follows:

\[
F_{s_1} (\theta; x, t) = \begin{cases} 
\int_0^\infty \Pi_k H(x_{L} - x) P_L(u) du, S_{wi} \leq \theta < S_L^{**} \\
\int_0^\infty \Pi_k H(x - x_{L}) P_L(u) du, S_L^{**} \leq \theta \leq S_D' \\
\int_0^\infty \Pi_k H(x - x_{L}) P_L(u) du, S_L^{**} < \theta \leq 1 - S_{wi} \\
\int_0^\infty \Pi_k H(x - x_{L}) P_L(u) du, S_D' \leq \theta \leq S_R^{**}
\end{cases}
\]  

(39)

This relation is subsequently expanded as shown below for the four distinct saturation segments. For \( x < x_{L}^{**}, S_{wi} < \theta < S_L^{**} \), we formulate the CDF as outlined in Equation C10, leading to:

\[
F_{s_1} (\theta; x, t) = H(\theta - S_B) \left( F_U \left( \frac{x}{f'(S_R^{*})} \right) - F_U \left( \frac{x}{f'(\theta)} \right) \right) \\
+ H(\theta - S_{wi}) \left( 1 - F_U \left( \frac{x}{f'(\theta)} \wedge \frac{x}{f'(S_R^{*})} \right) \right)
\]  

(40)

When \( x_{L}^{**} < x < x_{ir}^{*}, S_L^{**} \leq \theta \leq S_D' \), we define \( F_{s_1} (\theta; x, t) \) for the left branch, derived in Equation C11 as follows:

\[
F_{s_1} (\theta; x, t) = H(\theta - S_B) \left( F_U \left( \frac{x}{f'(S_R^{*})} \right) - F_U \left( \frac{x}{f'(\theta)} \right) \right) \\
+ H(\theta - S_{wi}) \left( 1 - F_U \left( \frac{x}{f'(\theta)} \wedge \frac{x}{f'(S_R^{*})} \right) \right)
\]  

(41)

For \( x_{ir}^{*} < x < x_{ir}^{*}, S_D' \leq \theta \leq S_R^{**} \), we define \( F_{s_1} (\theta; x, t) \) for the right branch, derived in Equation C13 as follows:

\[
F_{s_1} (\theta; x, t) = F_{s_1} (\theta; x, t) \\
+ H(\theta - S_{wi}) \left( 1 - F_U \left( \frac{x}{f'(\theta)} \wedge \frac{x}{f'(S_R^{*})} \right) \right)
\]  

(42)
The PDF of water saturation accurately captures discontinuities and shocks in the solution. at cell interfaces by solving a Riemann problem, and finding the fluxes between adjacent cells. This approach multiple shocks interacting with each other, such as the pure gravity segregation examined in our study. The of horizontal displacement, our approach employs the Godunov scheme to facilitate the numerical handling of data points on the resulting PDFs and subsequently the CDFs, we found that of data points, we can control the bandwidth. After conducting experiments to assess the impact of the number of value that balances smoothing and captures transitions from shock to rarefaction zones. By adjusting the number of smoothing applied to the density estimate. Very small bandwidth values lead to under-smoothed curves with much of the underlying structure. Achieving accurate CDF plots requires selecting an appropriate bandwidth value that balances smoothing and captures transitions from shock to rarefaction zones. By adjusting the number of data points, we can control the bandwidth. After conducting experiments to assess the impact of the number of data points on the resulting PDFs and subsequently the CDFs, we found that \( n = 2^7 \) is the reasonable range.

Given the CDF of saturation, the first two statistical moments of saturation read,

\[
\langle S_w(x, t) \rangle = 1 - \int_0^1 F_{S_x}(s) ds
\]

\[
\sigma^2_{S_w}(x, t) = 1 - \int_0^1 F_{S_x}(\sqrt{s}) ds - \langle S_w(x, t) \rangle^2
\]

Figure 7 represents a reasonable prediction for CDF of saturation at \( t_1, t_2 \) (before reflection), while at \( t_3, t_4 \) (after reflection) the CDF of saturation obtained from Equations 40 and 43, don’t capture the solution of MC scheme.

4. Numerical Experiments

4.1. Setting

In this section, we will compare the relationships derived for \( F_s(\theta; x, t) \) in Section 3 with the corresponding \( F_s(S, x, t) \) obtained from MC simulations of Equation 1 for the horizontal and updip displacement, and Equation 7 for the downdip displacement and the inverted gravity column. We will present the influence of parametric uncertainty on saturation uncertainty, by inspecting the mean, the variance, the temporal evolution of the CDF and PDF of water saturation at a specific location, the spatial evolution of the CDF and PDF of water saturation at a specific point in time, and the pointwise average of the CDFs generated at all locations along the domain, at a specific point in time. The aforementioned profiles are all computed using MCS as our reference solutions and the CDF method.

For the MC simulation of the nonlinear hyperbolic conservation laws (Equations 1 and 7), with complex initial and boundary conditions, one must generally resort to numerical schemes like finite element, finite difference, or finite volume approaches. We utilize the mass conservative finite volume discretization of the dimensionless form of Equations 1 and 7 in one-dimension. While prior studies (Ibrahima & Tchelepi, 2017; Ibrahima et al., 2015, 2018), have relied on a Lagrangian streamline simulation approach to handle the numerical treatment of horizontal displacement, our approach employs the Godunov scheme to facilitate the numerical handling of multiple shocks interacting with each other, such as the pure gravity segregation examined in our study. The Godunov scheme is an upwinding-type finite volume front-tracking method, which approximates the solution at cell interfaces by solving a Riemann problem, and finding the fluxes between adjacent cells. This approach accurately captures discontinuities and shocks in the solution.

The PDF of water saturation \( f_s(S_x) \) is generated using Kernel Density Estimation (KDE) (Botev et al., 2010). The CDF reflects the cumulative probability of a parameter being equal to or smaller than a given value. Hence, after generating the PDFs of uncertain input parameters using KDE, we utilize the resulting PDFs to calculate the CDFs through numerical integration. To achieve this, the Discrete Cosine Transform is employed (Botev et al., 2010). For the KDE of the PDF of random input parameters, we base our estimation on 10,000 samples of each random variable, assuming a Gaussian kernel, while allowing the bandwidth parameter to be automatically determined (Botev et al., 2010). The uniform discretization of the data for PDF estimation uses a mesh of \( n = 2^{10} \) points. The choice of bandwidth, or smoothing parameter, impacts the kernel’s width and affects the level of smoothing applied to the density estimate. Very small bandwidth values lead to under-smoothed curves with excessive spurious data artifacts. Conversely, larger bandwidth values result in over-smoothed curves that obscure much of the underlying structure. Achieving accurate CDF plots requires selecting an appropriate bandwidth value that balances smoothing and captures transitions from shock to rarefaction zones. By adjusting the number of data points, we can control the bandwidth. After conducting experiments to assess the impact of the number of data points on the resulting PDFs and subsequently the CDFs, we found that \( n = [2^7, 2^{12}] \) is the reasonable range.

Figure 3 represents spatiotemporal evolution of the average saturation fields and development of the shocks for each case study using the MC scheme.
We will present the results for three distinct cases: one with randomness solely in $\phi(x)$, another with randomness exclusively in $q(t)$, and a third case where both $\phi(x)$ and $q(t)$ are stochastic fields. It is worth mentioning that $F_{q(x,t)}(x,t)$ becomes a function of time only, that is, $F_{q(t)}(t)$, when the injection flux $q(t)$ is the sole source of uncertainty. Similarly, it becomes a function of space only, like $F_{\phi(x)}(x)$, when the porosity field $\phi(x)$ is the sole source of uncertainty. For cases where both fields are random, it becomes a space-time dependent function. The random porosity field has been restricted to the range $[0.3, 0.6]$, and the stochastic injection flux has been established to vary within the range $[0.3, 0.8]$, as depicted in Figure 4.

All cases have employed the Brooks-Corey expressions for the relative permeabilities as a function of saturation. We will demonstrate all the experiments for $m = 0.5$, which was formerly studied in test cases of Ibrahima et al. (2015), Ibrahima and Tchelepi (2017), and Zhang and Tchelepi (1999). The irreducible wetting and non-wetting saturations are assumed to be $S_{wi} = S_{oi} = 0.1$. The injection, if present, always happens at the inlet of the domain, that is, $x = a$. The final simulation time is $T = 1$ for all cases, except in the gravity column simulation, where it is set to $T = 10$.

4.1.1. Case 1: Stochastic Porosity Field $\phi(x)$

In the present scenario, we treat the injection flux $q_I(t)$ at the boundary as a fixed deterministic constant, specifically set at $q_{inj} = 0.3$. Hence, the random porosity field $\phi(x)$, is the sole source of uncertainty, and is characterized

![Figure 3](image1)

**Figure 3.** Spatiotemporal evolution of the deterministic saturation field represents the development of shock(s), (a) a single shock caused by horizontal flooding, (b) two shocks resulting from downdip flooding, (c) the reflection of two shocks from the boundaries in an inverted gravity column. The initial discontinuity in the downdip and gravity column cases is located at $Z_d = 0.3$.

![Figure 4](image2)

**Figure 4.** Multiple realizations of the (a) random porosity field and (b) random injection flux with the parameters defined in Section 4.1.3.
by its known mean, variance, covariance structure, and dimensionless correlation length. Following a methodology similar to Section 4.3.1 of Ibrahima et al. (2015), we introduce a random Gaussian field \( \gamma(x) \sim \mathcal{N}(\mu_x, C_{\gamma}(x)) \) to uphold the physical constraint \( 0 < \phi(x) < 1 \). Here, \( \mu_x \) denotes the mean, and \( C_{\gamma}(x) \) is an exponential covariance structure given by \( C_{\gamma}(x) = \sigma_\gamma^2 \exp\left(-\frac{x}{\lambda_\gamma}\right) \), where \( \sigma_\gamma^2 \) represents the variance of \( \gamma \), and \( \lambda_\gamma \) represents the correlation length. Subsequently, we define the porosity field as:

\[
\phi(x) = 0.01 \frac{1}{\pi} \arctan(\gamma(x)) + 0.5 \left(1 - \frac{2}{\pi} \arctan(\gamma(x))\right)
\]  

(46)

In consequence, we can choose \( \mu_x \) so that \( \langle \phi(x) \rangle = \mu_\phi \).

Further details about this setup can be found in Section 4.3.1 of Ibrahima et al. (2015).

Throughout our experiments with a stochastic porosity field, unless otherwise stated, we use \( \mu_\phi = 0.3, \sigma_\phi^2 = 0.5 \), and \( \lambda_\phi = 0.5 \) \( L \) where \( L = 1 \) is the dimensionless length of the domain. Figure 7 illustrates the outcomes where the random porosity field is the single source of uncertainty. Note that the vertical shock regions in the saturation profiles correspond to the horizontal regions in the CDF plots. As these plots demonstrate, our proposed method of distributions accurately matches the behavior of MC for the mean, standard deviation, and CDF of saturation.

As depicted in Figures 6 and 7, the proposed method accurately captures the behavior of the mean, the standard deviation, and the pointwise CDF of saturation across the domain in all the previous examples. However, it deviates from the reference solutions after the shocks are reflected, as shown in Figure 7. This is attributed to the complex dynamics of the wave interactions, which is not accurately captured by the method of characteristics.

### 4.1.2. Case 2: Stochastic Injection Flux \( q(t) \)

Enforcing the general continuity constraint for incompressible flow, \( \nabla \cdot q_x(x, t) = 0 \) makes the total flux \( q_x \) to be constant in \( x \), and is therefore equal to the injection flow rate at the left boundary of the domain, that is \( q_x(x, t) = q(t) = q_0(t) \). We are interested in finding the solutions to Equation 1 while treating \( q_0(t) \) as a stochastic field in time with a prescribed CDF. Henceforward, we opt to maintain porosity as a deterministic constant \( (\phi = 0.3) \) for this scenario. Thus, we focus solely on investigating the impact of randomness in the injection flux.

In order to find the distribution for the random injection flux at the inlet, similarly to the previous case, we assume the mean \( \mu_q \), variance \( \sigma_q^2 \), covariance structure \( C_q(t) \), and correlation time \( \tau_q \) are all known parameters. To this end, similarly to Ibrahima et al. (2015), we first define a Gaussian random field \( \rho_q(t) \sim \mathcal{N}(\mu_q, C_q(t)) \), with an exponential covariance structure \( C_q(t) = \sigma_q^2 \exp\left(-\frac{t}{\tau_q}\right) \), where \( \tau_q \) is the correlation parameter for events that are closer in time. Eventually, we define the stochastic injection flux field as,

\[
q_t(t) = 0.05 + 0.1(\rho_q(t))^2
\]  

(47)

Such a definition allows us to first make sure that \( q(t) > 0 \) and second by controlling \( \mu_q \), we can satisfy the criteria \( \langle q(t) \rangle = \mu_q \). Any other arbitrary non-negative distribution could be used alternatively.

Further details about this setup can be found in Section 4.2.1 of Ibrahima et al. (2015).

Unless otherwise stated, whenever experimenting with uncertainty in \( q(t) \), we will use \( \mu_q = 0.3, \sigma_q^2 = 0.5, \tau_q = 0.5 \) \( T \), \( T = 1 \), \( m = 0.5 \). Figure 6 show the results for the injection flux as the sole source of randomness.

### 4.1.3. Case 3: Uncertainty in Both \( \phi(x) \) and \( q(t) \)

In this section, we will illustrate the joint effects of uncertainty in the porosity field as well as the injection flux. We will resort to the same setup as the two previous sections for the construction of \( \phi(x) \) and \( q(t) \) fields. As for the numerical parameters, we will employ \( m = 0.5, \mu_x = 0.3, \sigma_x^2 = 0.5, \tau_x = 0.5 \) \( T \), \( T = 1 \), \( \mu_\phi = 0.3, \sigma_\phi^2 = 0.5, \lambda_\phi = 0.5 \) \( L \). Figure 4 illustrates four random sampling of the porosity field as well as the injection flux field plotted using the aforementioned values for mean, variance, and correlation length/time for each random variable.

In this section, we will illustrate the joint effects of uncertainty in the porosity field as well as the injection flux, as depicted in Figure 5. We will encapsulate both uncertainties in the structure of the stochastic velocity field by representing it as \( v_t = v_t(x, t) \).
5. Comparison With Low-Order Approximation

In the previous section, we demonstrated that the proposed CDF method provides accurate approximations of the mean, standard deviation, and distribution functions of the saturation field. Both MCS and the CDF method determine saturation moments through a post-processing step by first finding $F_s(S_w, x, t)$ and then employing Equations 44 and 45 to compute the first two moments of saturation. In contrast, SME methods, also referred to as LOA, utilize perturbation expansions of the stochastic input fields to directly calculate the two leading moments of saturation. In this section, we compare the proposed CDF method with a specific LOA approach, while considering MCS as our reference solution. Following the methodology of Ibrahima et al. (2015) and Zhang and Tchelepi (1999), we will investigate how the solutions obtained from the CDF method and the LOA approach deviate from the outcomes of the MCS as we alter the variance and correlation length of the underlying stochastic porosity and/or injection flux.

Figure 5. (First row) The first two moments of saturation, (second row) spatial and temporal evolution of the cumulative distribution function (CDF) of saturation (dashed lines show the results of the method of distributions, and solid lines correspond to Monte Carlo (MC) simulations), (third row) pointwise average of the CDF and probability density function at all points along the domain, obtained from both MC and CDF methods. All simulations represent horizontal case with $\phi(x)$ random, $\mu_\phi = 0.3$, $\sigma_\phi^2 = 0.5$, $\lambda_\phi = 0.5$, $L = 1$, and $q(t)$ random, $\mu_q = 0.3$, $\sigma_q^2 = 0.5$, $\tau_q = 0.5$, $T = 1$. Solid lines represent the results of MC simulations, while dashed lines represent the results of the CDF method.
5.1. Formulation

In this section, we follow the exact same setup as in Section 4.5.1 of Ibrahima et al. (2015). First we assume a deterministic constant porosity \( \phi = \phi_0 = 0.3 \), and a lognormally distributed injection flux \( q \), with \( \mu_q = 0.3 \) and standard deviation \( \sigma_q \) as follows:

\[
q \sim \log \mathcal{N}(\langle \ln(q) \rangle, \sigma_{\ln(q)}) \quad \langle \ln(q) \rangle = \ln\left( \frac{\mu_q^2}{\sigma_q^2 + \mu_q^2} \right), \quad \sigma_{\ln(q)} = \sqrt{\ln\left( \frac{\sigma_q^2}{\mu_q^2} + 1 \right)}
\]  

(48)

Utilizing the concept of displacement along a streamline, we define \( \tau(x; x_0) \) as the travel time (time of flight) of a particle to move from \( x_0 = 0 \) to \( x \) within the total velocity field \( v_r \), as per Zhang and Tchelepi (1999):

\[
\frac{d\tau}{dx} = \frac{1}{v_r} = \frac{\phi_0}{q}
\]  

(49)

Figure 6. (First row) The first two moments of saturation, (second row) spatial and temporal evolution of the cumulative distribution function (CDF) of saturation (dashed lines show the results of the method of distributions, while solid lines correspond to Monte Carlo (MC) simulations), (third row) pointwise spatial average of the CDF and probability density function at all points along the domain, obtained from MC and CDF methods. All plots correspond to the downdip flooding with \( q(t) \) random, \( \mu_q = 0.3, \sigma_q = 0.5, \tau_q = 0.5 \ T, \phi = 0.3 \), at two dimensionless times \( t_1 = 0.2, t_2 = 0.3 \).
Since $v_T$ is random, so is $\tau$, and hence, its statistical moments depend on those of $v_T$. After some mathematical manipulations as detailed in Ibrahima et al. (2015), and assuming a lognormal distribution for $\tau$ as $\tau \sim \log \mathcal{N}(\langle \ln(\tau) \rangle, \sigma_{\ln(\tau)})$, the corresponding moments are defined as follows (Zhang & Tchelepi, 1999):

$$\langle \ln(\tau) \rangle = 2\ln(\langle \tau \rangle) - \frac{1}{2} \ln[\langle \tau^2 \rangle + \sigma_{\ln(\tau)}^2]$$

$$\sigma_{\ln(\tau)}^2 = \ln[\langle \tau^2 \rangle + \sigma_{\ln(\tau)}^2] - 2\ln(\langle \tau \rangle)$$

Subsequently, the first-order estimate of the ensemble mean and standard deviation of water saturation is formulated as follows:

$$\langle S_w(x,t) \rangle = \int_0^{+\infty} \bar{S}(\tau,t)p_\tau(\tau;x,x_0)d\tau, \quad \sigma_{S_w}^2(x,t) = \int_0^{+\infty} \bar{S}^2(\tau,t)p_\tau(\tau;x,x_0)d\tau - \langle S(\tau,t) \rangle^2$$

Figure 7. (First row) The first two moments of saturation (solid lines are the results of Monte Carlo (MC) simulations, while dashed lines show the corresponding deterministic solutions, and markers show the results of the method of distributions), (second/third row) the spatial and temporal evolutions of the cumulative distribution function (CDF) of saturation at four fixed dimensionless times, $t_1 = 0.6$, $t_2 = 1.2$, $t_3 = 4.5$, $t_4 = 7.5$, and at dimensionless spatial positions along the domain, temporal evolution of the CDF of saturation at a fixed dimensionless spatial position along the domain (dashed lines show the results of the method of distributions, while solid lines correspond to MC simulations), (fourth row, left) the temporal evolution of the CDF of saturation at a fixed dimensionless position ($x = 0.7$) and at two dimensionless times, (fourth row, right) the pointwise spatial average of the CDF of saturation along the domain at four dimensionless times. All simulations represent an inverted gravity column with $\phi(x)$ random, $\mu_\phi = 0.3$, $\sigma_\phi = 0.5$, $\lambda_\phi = 0.6$, $L = 3$, $q = 0.3$. Except in the saturation profile, solid lines show the results of MC, while dashed lines are the result of the CDF method.
where \( p_f(\tau; x, x_0) \) is the PDF of the travel time \( \tau \), and \( \dot{S}(\tau, t) \) is found by combining Equations 1 and 49, resulted in a transformed version of the transport equation as follows:

\[
\frac{\partial \dot{S}}{\partial t} + f'w(S) \frac{\partial \dot{S}(\tau, t)}{\partial \tau} = 0
\]  
(52)

where we consider the inclusion of gravitational effects in the flux function when solving Equation 52.

In the second scenario, we assume a constant deterministic injection flux \( q = q_0 = 0.3 \), and a random stationary Gaussian porosity field \( \phi(x) \) characterized by its mean value of \( \mu_\phi = 0.3 \), and covariance structure \( \Sigma_\phi(x) = \sigma_\phi^2 \exp\left(-\frac{|x|}{\lambda_\phi}\right) \). Subsequently, the first-order approximation of the first two moments of \( \tau \) are formulated as follows (Zhang & Tchelepi, 1999):

\[
\langle \tau(x; x_0) \rangle \approx (x - x_0) \frac{\mu_\phi}{\phi_0}, \quad \sigma_\tau^2(x; x_0) \approx \frac{2\sigma_\phi^2}{q_0^2} \lambda_\phi (x - x_0) - \lambda_\phi^2 \left(1 - \exp\left(-\frac{|x - x_0|}{\lambda_\phi}\right)\right)
\]  
(53)

By controlling \( \mu_\phi^\prime, \lambda_\phi^\prime \) and \( \sigma_\phi^\prime \), we will provide comparisons between the first two moments of water saturation from LOA and those obtained from MCS and the CDF method.

### 5.2. Illustrative Examples and Numerical Results

As depicted in Figure 9, while the results from the CDF method remain consistent with those of MCS even for large variance and correlation lengths, the accuracy of LOA starts declining even for small variances. This occurs because statistical moments of the travel time and velocity are approximated as first-order, requiring log permeability variance to be much smaller than unity. As depicted in Figure 9, by increasing the variance of input parameters, the saturation variance increases as well. Consequently, the saturation profile becomes smoother and deviates from the sharp deterministic profile in the shock region. Figure 8 demonstrates the results of sensitivity analysis to the correlation length. Initially, the LOA results are far from their MCS and CDF counterparts. As we increase the correlation length while keeping \( \Delta x \) constant, the approximations for both mean and standard deviation become closer to those of MCS. This is because more grid blocks fall within one correlation length, and hence, the underlying domain becomes more homogeneous to resolve. Furthermore, as shown in Figure 9, when dealing with scenarios involving two shocks, LOA struggles to differentiate between the shocks during the early stages, often predicting a single combined shock, unless variances are extremely small. In contrast, the CDF method consistently and accurately captures MCS solutions both in the initial and later time periods.

### 6. Accuracy and Efficiency of the CDF Method

For the MC simulations of the BL equation, \( N_{MC} = 3,000–5,000 \) were sufficiently adequate for the mean and standard deviation profiles to converge, with a grid size of \( \Delta x = 5e - 4 \), \( \Delta t = 1e - 2 \). Also, a large number of realizations were essential for the CDF plots to be smooth. The convergence of our proposed CDF expressions to the reference MCS solutions relies on accurately estimating the CDF of the random input parameters. This involves generating a substantial number of realizations for the underlying random fields, computing their PDF using KDE, and subsequently deriving the CDF of uncertain inputs. To achieve a close alignment between \( F_\theta(\theta; x, t) \) obtained through our proposed method and the reference MC solutions, we determined that utilizing around \( N = 1,000 – 3,000 \) realizations of the random input was sufficient.

As depicted in Figure 10, by increasing the number of MC samplings, the \( L_2 \) norm of the difference between the saturation CDFs from our CDF method and the reference MCS will keep declining up to \( N_{MC} = 5,500 \), at which an error of 0.08 is observed. Beyond this point, further increases in the number of trials does not result in a noticeable decrease in the error. The \( L_2 \) norm errors in the sensitivity studies presented in Figures 10, 12, and 13 are usually bounded by 0.1 for spatial and temporal grid sizes of order \( 1e - 3 \) and \( N_{MC} \approx 5e3 \). While this error for the CDF of water saturation in accuracy studies of the Buckley-Leverett problem is reported to be reasonable (Fuks et al., 2019), other metrics such as the averaged Wasserstein distance might need to be constrained to smaller values to demonstrate accuracy when comparing the disparities between CDFs from the distribution method and the baseline MCS.
Assuming that we are comparing our CDF solutions to a baseline MC simulation generated with large enough number of realizations and very fine spatial/temporal grids, then, any deviation of the semi-analytical CDF solutions from the MC results would likely be attributable to either insufficiently small spatial/temporal grid sizes of the random input parameters or an insufficient number of realizations when generating samples of these underlying random fields. In addition to grid sizes and sample counts, it should be noted that our CDF method relies on generating the PDFs of random inputs using KDE. Therefore, we make certain assumptions in this process, including the use of a Gaussian kernel for KDE generation of the PDFs of random inputs ($f_U(t(x))$). This choice may not fully represent the underlying distribution, particularly in cases involving correlations and multi-modal underlying distributions. We also rely on automatic bandwidth selection, as in Botev et al. (2010). Furthermore, when finding CDFs, we rely on approximating the numerical integration of PDFs using discrete cosine transform. Besides these assumptions and approximations, it is worth mentioning that the CDF formulation does not impose any prior assumption on the number of random parameters or their correlation structure (Cheng et al., 2019).

Figure 8. Approximations of the first two moments from the low-order approximations, Monte Carlo simulations and the cumulative distribution function methods for the horizontal flooding with $\phi(x)$ random at dimensionless times $t_1 = 0.15$, $t_2 = 0.25$. For all cases, $\sigma_\phi^2 = 10^{-3}$, $\Delta x = 0.005$, $\Delta t = 0.01$, while the correlation length is increasing as $\lambda_\phi = 0.01, 0.05, 0.5, 0.7$ from top to bottom rows.
Regarding efficiency, our method is usually two orders of magnitude faster than the corresponding MCS experiment. The most time-consuming part of our CDF method is generating the PDFs of the input random fields, that is, using KDE to find the PDFs of random inputs, followed by finding the corresponding CDFs \( F_U(t|\mathbf{x},t) \). However, this process is still considerably faster than the MCS approach, which involves generating 5,000 samples of the stochastic input fields, solving the nonlinear Buckley-Leverett equation using the Godunov method, and then using KDE to post-process the resulting saturation field and find the saturation PDFs and subsequently the CDFs \( F_S(S_w,\mathbf{x},t) \). Once the CDFs of the underlying random fields are generated in our CDF method, there is no computational cost associated with our proposed semi-analytical CDF methodology for computing \( F(S_w,\mathbf{x},t) \). Therefore, the CDF method is consistently much faster than the baseline MCS scheme.

Figure 9. Approximations of the first two moments from the low-order approximation (LOA), Monte Carlo (MC) simulations and the cumulative distribution function (CDF) method for the downdip flooding with \( q(t) \) random, and \( \sigma_q = 0.005, 0.01, 0.02, 0.05, 0.1 \) from top to bottom rows. For all cases, we consider \( \mu_q = 0.3, \tau_q = 0.5 \text{T}, \) and \( T = 1 \). As variance increases, LOA estimates of the first two moments deteriorate, whereas CDF results stay in agreement with the corresponding MC solutions.
The convergence study conducted to assess the accuracy of the Godunov solver used in the reference MC solutions of Equations 1 and 7 is presented in Figure 11. The temporal grid size is maintained at a constant value of $\Delta t = 1 e^{-3}$, while experimenting with spatial grid sizes of $\Delta x = 1 e^{-2}, 1 e^{-3}, 5 e^{-3}, 1 e^{-4}$. The solution with the finest grid size ($\Delta x = 1 e^{-4}$) serves as the reference, and the plots depict the $L_2$ norm of the difference between the reference solution (using the finest grid size) and the solutions with the other mentioned grid sizes. As anticipated, the results exhibit a first-order accuracy in $\Delta x$, consistent with the discretization method employed in the numerical implementation of the Godunov scheme. A similar procedure is followed with a fixed spatial grid size, but varying time step sizes. In this analysis, time steps of $\Delta t = 2 e^{-3}, 1.7 e^{-3}, 1.4 e^{-3}, 1 e^{-3}$ are considered, while keeping $\Delta x = 1 e^{-3}$ constant. The solution with the smallest time step is utilized as the reference, and the plots illustrate the $L_2$ norm of the difference between the reference solution and the solutions with the other mentioned time steps. The results exhibit closer-to-second-order accuracy in terms of $\Delta t$.

7. Sensitivity to the Input Uncertainty

The $L_2$ norm error of the average $F_s(S, x, t)$ along the domain, obtained from the CDF method and the reference MCS are shown in Figures 12 and 13 for different statistical properties, such as variance and correlation length. Figure 12 demonstrates that the error declines with time. Additionally, increasing either the correlation time or the variance increases the error, as anticipated. In Figure 13, when experimenting with the sensitivity of $F_s(s)$ to the correlation length/time of the input stochastic fields, lower error is observed for $\lambda_{\phi} > 0.5$. This is because more blocks fall within one correlation length/time and hence the solution becomes more homogeneous to resolve. Additionally, according to Figure 12, setting the correlation time $\tau_q(t) < 0.5$ threshold results in lower error compared to higher values of correlation time. Overall, errors are usually bounded by 0.1 for the grid sizes $\Delta x = 1e^{-3}, \Delta t = 1 e^{-2}$ when experimenting with the sensitivity to the input uncertainty. As expected, a tradeoff exists between computational efficiency and accuracy. While employing smaller grid sizes, especially $\Delta x$, could result in reduced errors, this would significantly extend the runtime of the MCS. Also, while experimenting with the values of variances of both input random fields, as Figure 13 represents the highest error observed when both variances are high.

8. Summary and Conclusions

We developed a semi-analytical CDF methodology for probabilistic forecast of immiscible two-phase transport in heterogeneous porous media for vertical domains. We considered one-dimensional problem with an uncertain

![Figure 10](image-url)  
*Figure 10. $L_2$ norm error between the average cumulative distribution functions (CDFs) of saturation along the domain obtained from the CDF method and the reference Monte Carlo simulations, as a function of the Monte Carlo trials. This experiment employs a constant $\Delta x = 0.001$, and $\Delta t = 0.01$.*

![Figure 11](image-url)  
*Figure 11. Convergence study for the Godunov solver used in the Monte Carlo reference solutions of the Buckley-Leverett equation. (a) obtained with a constant $\Delta t = 10^{-3}$ and varying spatial grid sizes, and (b) obtained with a constant $\Delta x = 10^{-3}$ and varying temporal grid sizes.*
space-dependent porosity field within the domain, and a random time-varying injection flux at the inlet boundary, while incorporating buoyancy forces which lead to multiple shocks and rarefaction zones. This method addresses spatiotemporal characteristics beyond single-shock scenarios.

As described, the method of distributions propagates uncertainty from random input parameters to the output state variable by converting the stochastic nonlinear Buckley-Leverett equation into a linear deterministic equation for the fine-grained CDF of saturation. This encapsulates uncertainty in the equation’s coefficients, making the problem more tractable. We solved this resulting linear equation using the method of characteristics. We derived exact expressions for saturation CDFs, avoiding approximations and preserving the physics, particularly the presence of shocks in the solution. Building upon the approach of Ibrahima and Tchelepi (2017) for mapping CDFs, our methodology directly quantifies uncertainty by initially establishing the CDF of random inputs, denoted as \( F_U(x, t) \), and then employing our proposed analytical expressions for \( F_s(\theta; x, t) \) to compute the saturation CDFs.

We developed our CDF methodology by extending a previous study (Wang et al., 2013) that focused on horizontal reservoirs with random injection flux as the only source of uncertainty. We focused on converting nonlinear stochastic hyperbolic conservation laws into deterministic expressions for saturation CDFs, accounting for the presence of multiple shocks.

We conducted MC simulations of the nonlinear Buckley-Leverett equation using the Godunov scheme. Subsequently, we performed a series of numerical experiments to validate our CDF methodology for various test cases and physical scenarios. This scenarios included horizontal flooding, updip flooding, downdip flooding, and pure

![Figure 12](image12.png)

**Figure 12.** Sensitivity to the correlation length and variance of the input random variable. \( L_2 \) norm error of the cumulative distribution function (CDF) of saturation computed at two specific dimensionless times \( t_1 = 0.6, t_2 = 1.5 \), using the reference Monte Carlo simulations and the CDF method, for \( q(t) \) as the sole source of uncertainty.

![Figure 13](image13.png)

**Figure 13.** \( L_2 \) norm error of the cumulative distribution function (CDF) of saturation computed at an early time \( t = 0.6 \), using reference Monte Carlo simulations and the CDF method, for the test cases with both \( \phi(x) \) and \( q(t) \) random. Sensitivity to the correlation length/time and variances of both input random variables demonstrates accuracy of our CDF method.
gravity segregation in an inverted gravity column. We addressed the unique characteristics of rarefaction zones and shocks in each case. Our study leads to the following conclusions:

- The accuracy of our proposed method relies on accurately estimating the CDFs of the random input parameters. This involves generating a substantial number of realizations for the underlying random fields, computing their PDFs using KDE, and subsequently deriving the CDFs of uncertain inputs. Despite the need for a significant number of realizations to generate PDFs (and subsequently CDFs), the computational efficiency of the CDF method surpasses that of MCS for the nonlinear Buckley-Leverett equations.

- We studied this problem for a random injection flux and/or a randomly correlated porosity field, considering a broad spectrum of correlation lengths and variances. Our results revealed that the CDFs obtained via the CDF method remain in agreement with reference MCS across a wide range of statistical properties of the random inputs. In contrast, the first-order approximations of the SME method deviate from the reference solutions, except for very small variances and correlation lengths.

- Our approach provides a pointwise probabilistic description of saturation, enabling the exploration of distribution tails—higher-order moments like skewness and kurtosis—that are pivotal for risk assessment.

- A comprehensive error analysis confirmed the robustness of the developed method in this work.

- Extending this work to higher dimensions involves manipulating the interaction of waves in multiple dimensions by introducing a kinetic defect term to the linear equation of the fine-grained CDF. This addition ensures the satisfaction of the entropy condition in all dimensions.

**Appendix A: Derivation of the Two-Phase Hyperbolic Conservation Law**

The two-phase extension of the single-phase Darcy’s law for water and oil phases leads to:

\[
\begin{align*}
\mathbf{u}_m &= \frac{k k_{rm}}{\mu_w} \nabla \phi_w = \frac{k k_{rm}}{\mu_w} \nabla (P_w + \rho_w g) = -\frac{k k_{rm}}{\mu_w} \nabla (P_w - P_o + \rho_w g \nabla h) \quad \text{(A1)} \\
\mathbf{u}_o &= -\frac{k k_{ro}}{\mu_o} \nabla \phi_o = -\frac{k k_{ro}}{\mu_o} \nabla (P_o + \rho_o g) = -\frac{k k_{ro}}{\mu_o} \nabla (P_o + \rho_o g \nabla h) \quad \text{(A2)}
\end{align*}
\]

where capillary pressure relates the pressures of two phases as \( P_w(S_w) = P_o - P_c \). \( \mathbf{u}_\alpha (\alpha = \{w, o\}) \) are the phase Darcy velocities of the water and oil phases. \( k_{rm}, \mu_\alpha \) and \( \rho_\alpha (\alpha = \{w, o\}) \) represent relative permeability, viscosity and density of each phase, respectively. In the case of vertical reservoirs, \( h \) is the elevation relative to a reference depth. Applying mass conservation on a control volume results in the transport equation (saturation equation):

\[
\phi(x) \frac{\partial S_\alpha}{\partial t} + \nabla \cdot \mathbf{u}_\alpha = 0 \quad \text{for } \alpha = \{w, o\} \quad \text{(A3)}
\]

where the phase saturations, \( S_w \) and \( S_o \) are the volume fraction of the pore space occupied by the corresponding fluid phase. Consequently, \( S_w + S_o = 1 \) simplifies the two mass conservation equations for the water and oil phases, to the incompressibility condition of \( \nabla \cdot \mathbf{u}_\tau = 0 \) for total Darcy flux. Subsequently, we obtain an equation in terms of pressures:

\[
\mathbf{u}_\tau = \mathbf{u}_w + \mathbf{u}_o = -\lambda_T \nabla P_w + \lambda_o \nabla P_o - (\lambda_o \rho_o + \lambda_w \rho_w) g \nabla h \quad \text{(A4)}
\]

where the relative mobilities are defined as \( \lambda_\alpha = \frac{k k_{rm}}{\mu_\alpha} (\alpha = \{w, o\}) \) for each phase and the total mobility reads \( \lambda_T = \lambda_w + \lambda_o \). The three terms on the right-hand side of Equation A4 represent viscous, capillary and buoyancy forces, respectively. The dimensionless flux function of the water phase, referred to as the fractional flow of water is defined as the water phase velocity divided by the total velocity:

\[
f_w = \frac{\mathbf{u}_w}{\mathbf{u}_\tau} = \frac{\lambda_w}{\lambda_T} \left( 1 + \frac{\lambda_o}{\lambda_T} (\nabla P_o - \Delta \rho g \nabla h) \right) \quad \text{(A5)}
\]

In the absence of capillarity, the two phase pressures are equal and identical to the global pressure. In such a scenario, we consider one-dimensional flow in an inclined reservoir with a constant dip angle \( \theta \), where \( 0 \leq \theta \leq 90 \),
ranging from 0 for horizontal reservoirs to 90 for vertical case studies, resulting in $N_g = \sin \theta$. The dimensionless gravity number $N_g$ is defined as the ratio of buoyancy to viscous forces:

$$N_g = \frac{kg(\rho_w - \rho_o)}{\mu_o \mu_e}$$  \hspace{1cm} (A6)

Subsequently, defining the viscosity ratio $m = \frac{\mu_o}{\mu_e}$, while employing the definitions for mobilities, the fractional flow of water can be recast as Equation 2. Rewriting the mass conservation of water saturation (Equation A3) using the fractional flow $f_w$, while applying the chain rule and incompressibility condition, leads to:

$$\frac{\partial S_w}{\partial t} + v_r(x, t) \cdot \nabla f_w(S_w) = 0$$  \hspace{1cm} (A7)

where $v_r(x, t)$ is defined as the interstitial velocity (total seepage velocity field) $v_r(x, t) = \frac{q^T(x, t)}{\phi(\mathbf{x})}$, where $q^T(x, t)$ is the total volumetric flow rate, obtained by multiplying the total Darcy velocity by the area A (In this study, A is assumed to be 1.). We define the total flux to be time-dependent. This is a feasible assumption because the incompressibility condition imposes $q_r(x, t)$ to be x-independent and hence equal to the injection flow rate at the inlet boundary which could be time-dependent. That is, $q_r(x, t) = q_r(x = 0, t) = q_{inj}(t)$. In this study, we assume the total velocity field $v_r(x, t)$ is a random variable, where its uncertainty arises from either or both sources/physical phenomena; the spatially-varying porosity field is uncertain in space, whereas the time-varying total flux is a random variable in time.

It should be noted that fractional flow $f(S_w)$ is a continuous smooth, and hence differentiable function. Utilizing the chain rule, we get $\nabla f_w(S_w) = f_w'(S_w) \nabla S_w$, where $f_w'(S_w) = \frac{\partial f_w(S_w)}{\partial S_w}$. Subsequently, supplemented with the following initial/boundary conditions, the Buckley-Leverett equation defines an initial boundary value problem for water saturation which is known to admit analytical solutions in terms of $\frac{S_w}{S_o}$, and is recast as Equation 1 in the scalar form.

In order to find the flux function for the pure gravity segregation case, we start with Equation A1 for the vertical velocity of water and oil. After rearranging and subtracting the two equations, and applying $u_w = -u_o$ in the absence of capillarity, we end up with:

$$u_w = \frac{g(\rho_w - \rho_o)k}{\mu_w} \frac{k_{re}}{1 + (k_{riw}/k_{roi})} \equiv u_o G(S_w)$$  \hspace{1cm} (A8)

where the first fraction is assumed to be a characteristic velocity resulting from gravity $u_o$, and the second fraction is the dimensionless flux function $G(S_w)$. Hence, fractional flow for pure gravity segregation is defined as $G(S_w) = \frac{2}{\mu_o}$, and is equal to Equation 6. Therefore, the one-dimensional transport equation is recast as Equation 7.

**Appendix B: Derivation of the Fine-Grained CDF Equation**

Starting with the definition of the stochastic fine-grained (raw) CDF function $\Pi(\theta; S_w; x, t) = H(\theta - S_w(x, t))$, we find its spatial and temporal derivatives as follows (Appendix A of Wang et al. (2013)):

$$\nabla \Pi = \frac{\partial \Pi}{\partial S} \nabla S = -\frac{\partial \Pi}{\partial \theta} \nabla S$$  \hspace{1cm} (B1)

$$\frac{\partial \Pi}{\partial t} = \frac{\partial \Pi}{\partial S} \frac{\partial S}{\partial t} = -\frac{\partial \Pi}{\partial \theta} \frac{\partial S}{\partial t}$$  \hspace{1cm} (B2)

For smooth solutions, multiplying Equation 1 with $\frac{\partial S}{\partial \theta}$ and substituting the temporal derivative above results in:

$$-\frac{\partial \Pi}{\partial t} + v_r(x) \frac{\partial \Pi}{\partial \theta} \cdot \nabla S = 0$$  \hspace{1cm} (B3)

Leveraging the property of the Heaviside function as $\frac{\partial \Pi}{\partial \theta} = \delta(\theta - s)$ leads to:

$$-\frac{\partial \Pi}{\partial t} + v_r(x) \delta(\theta - s) \cdot \nabla S = 0$$  \hspace{1cm} (B4)

Combining this expression with the property of the Dirac delta function $f(s) \delta(\theta - s) = f(\theta) \delta(\theta - s)$ results in:
$$\frac{\partial \Pi}{\partial t} + v_s(\theta) \frac{\partial \Pi}{\partial \theta} \cdot \nabla_{\theta} = 0$$  \hspace{1cm} (B5)

Finally, the spatial derivative of the raw CDF function in Equation B1 turns this equation into its final form:

$$\frac{\partial \Pi}{\partial t} + v_s(\theta) \cdot \nabla \Pi = 0$$  \hspace{1cm} (B6)

Unlike the saturation equation, this equation is linear and easier to handle.

**Appendix C: Derivation of the Water Saturation CDF Equations**

In this section, we present the derivation of the water saturation CDF, that is $F_s(\theta; x, t)$ equations for different scenarios. For the horizontal displacement, we commence with the first relation in Equation 31 which describes the CDF over $S_w < \theta < S^*$. After substituting the expression for $\Pi_0$ from relation (21), we integrate both sides of Equation 10. Next, we replace the expression for the front location $x$ in Equation 31 with $f'(S^*) \int_0^{t_f(\theta)} dt'$. Then, we utilize the definition of $U(x, t)$ from Equation 30. The transition from the second to the third line involves a change of variables in the integral and relies on the properties of the Heaviside step function. Specifically, $x - f(S^*)u > 0$ implies $\frac{x}{f(S^*)} > u$, which aligns with the argument of the Heaviside function in the third line. These steps are illustrated as follows:

$$F_{s_u}(\theta; x, t) = \int_0^\infty \Pi_u H(x - x_f) P_u(u) du$$
$$= H(\theta - S_{w1}) \int_0^\infty H(x - f'(S^*)u) P_u(u) du$$
$$= H(\theta - S_{w1}) \int_0^\infty H \left( \frac{x}{f(S^*)} - u \right) P_u(u) du$$
$$= H(\theta - S_{w1}) F_u \left( \frac{x}{f(S^*)} \right)$$  \hspace{1cm} (C1)

where the last derivation step was performed by applying Equation 18, leading to the relation for $F_s(\theta; x, t)$ in terms of the CDF of the random input field $U(x, t)$. The final expression in the last line is also provided in Equation 32. Expanding the second expression in Equation 31, we note that CDF is a cumulative quantity and hence, we aggregate $F_{s_u}(\theta; x, t)$ with the new term specific to the current saturation segment as outlined in the first line below. In the second line, we substitute the expression for $\Pi_0$ from Equation 24. Continuing the derivation, we replace the definitions of $C(\theta, x, t)$ and the front location ($x_f$) from Equations 26 and 10, respectively. The transition to the last line involves the same change of variables as in the previous derivation, where $x - f'(S^*)u > 0$ implies $\frac{x}{f(S^*)} > u$. These steps are presented below:

$$F_{s_u}(\theta; x, t) = F_{s_u}(\theta; x, t) + \int_0^\infty \Pi_u H(x - x_f) P_u(u) du$$
$$= F_{s_u}(\theta; x, t) + \int_0^\infty \left[ H(\theta - S_{w1}) H(x - C) H(x_f - x) + H(\theta - S_B) H(C - x) H(x_f - x) \right] P_u(u) du$$
$$= F_{s_u}(\theta; x, t) + \int_0^\infty \left[ H(\theta - S_{w1}) H(x - f'(\theta)u - x) H(f'(S^*)u - x) \right] P_u(u) du$$
$$= F_{s_u}(\theta; x, t) + \int_0^\infty \left[ H(\theta - S_{w1}) H \left( \frac{x}{f'(\theta)} - u \right) H \left( \frac{x}{f'(S^*)} - u \right) \right] P_u(u) du$$

$$+ H(\theta - S_B) H \left( \frac{x}{f'(\theta)} - u \right) H \left( \frac{x}{f'(S^*)} - u \right) P_u(u) du$$  \hspace{1cm} (C2)

Ultimately, using the following relations for the convolution of two Heaviside functions, the final form of this equation is recast as in Equation 33.

$$\int_0^\infty H \left( \frac{x}{f'(\theta)} - u \right) H \left( \frac{x}{f'(S^*)} - u \right) P_u(u) du = \int_{f'(\theta)}^{f'(S^*)} P_u(u) du = F_u \left( \frac{x}{f'(\theta)} \right) - F_u \left( \frac{x}{f'(S^*)} \right)$$  \hspace{1cm} (C3)
In the first integral of Equation C3, since the first Heaviside function is 1 when \( u < \frac{x}{f'(\theta)} \) and the second Heaviside function is 1 only when \( u > \frac{x}{f'(S^*)} \), the integral is non-zero only when both conditions are satisfied. This means \( u \) should be between \( \frac{x}{f'(\theta)} \) and \( \frac{x}{f'(S^*)} \). Accordingly, we adjusted the lower and upper limits of the integral. Finally, leveraging the properties of CDFs, the probability that \( U \) falls within an interval \([A, B]\) is given as follows:

\[
\int_{B}^{A} P_U du = F_U(A) - F_U(B) \tag{C4}
\]

Furthermore, we follow the same logic for the following convolution of two Heaviside functions. In order for the first line in Equation C4 to be valid, both conditions must be satisfied. That is, \( u > \frac{x}{f'(\theta)} \) and \( u > \frac{x}{f'(S^*)} \), requiring \( u > \max\left(\frac{x}{f'(\theta)}, \frac{x}{f'(S^*)}\right) \) or \( u > X \). This results in the adjusted integration bounds of \([X, \infty)\), as follows:

\[
\int_{0}^{\infty} H\left(u - \frac{x}{f'(\theta)}\right) H\left(u - \frac{x}{f'(S^*)}\right) P_U(u) du = \int_{X}^{\infty} P_U(u) du = 1 - F_U \left( \frac{x}{f'(\theta)} \lor \frac{x}{f'(S^*)} \right) \tag{C5}
\]

For the downdip displacement and the inverted gravity column before the waves rebound from the boundaries, we perform mathematical manipulations on each line of Equation 34. For \( x > x_{tr} \), \( S_{tr} < \theta < S^*_R \), we expand the first line in Equation 34 using the definition of \( \Pi_n \), and following a similar procedure as in Equation 1, but considering two fronts in this case. Thus, we replace \( x \) with \( x_{tr} = f'(S^*_R)U(x, t) \), corresponding to this saturation range. These steps are presented in Equation C6, ultimately leading to the equation in the last line, also provided in Equation 35.

\[
F_{n_{tr}}(\theta; x, t) = \int_{0}^{\infty} \Pi_n H(x - x_{tr}) P_U(u) du = H(\theta - S_{tr}) \int_{0}^{\infty} H(x - f'(S^*_R)u) P_U(u) du \]

\[
= H(\theta - S_{tr}) \int_{0}^{\infty} H\left(\frac{x}{f'(S^*_R)} - u\right) P_U(u) du \tag{C6}
\]

Applying Equation 18 on the last expression, we find the relation for \( F_{n_{tr}}(\theta; x, t) \) in terms of the CDF of the random input field \( U(x, t) \), resulting in the final expression as provided in Equation 35.

For \( x > x_{tr} \), \( S^*_R < \theta < S_D \), the derivation steps are outlined in Equation C7. We begin by utilizing the second line in Equation 34, where we combine the CDF of the current range with the CDF from earlier times for this right-moving wave, denoted as \( F_{n_{tr}}(\theta; x, t) \), and derived in Equation C6. The derivation steps are outlined below. The transition from the first to the second line involves utilizing the definition of \( \Pi_{tr} \) from Equation 25, relation 1. This is followed by replacing the definitions of \( C(\theta, x, t) \) and \( x_{tr} \) as before. Next, we apply a similar change of variable as before and leverage the properties of the Heaviside convolutions, as fully explained above. Ultimately, by applying Equation 18, we get the last line, also provided in Equation 36.

\[
F_{n_{tr}}(\theta; x, t) = F_{n_{tr}}(\theta; x, t) + \int_{0}^{\infty} \Pi_{tr} H(x_{tr} - x) P_U(u) du \]

\[
= F_{n_{tr}}(\theta; x, t) + \int_{0}^{\infty} \left[ H(\theta - S_{tr}) H(x_{tr} - x) + H(\theta - S_D) H(C - x) H(x_{tr} - x) \right] P_U(u) du \]

\[
= F_{n_{tr}}(\theta; x, t) + \int_{0}^{\infty} \left[ H(\theta - S_{tr}) H(x - f'(S^*_R)u) H(f'(S^*_R)u - x) \right] P_U(u) du \]

\[
+ H(\theta - S_D) H\left(\frac{x}{f'(\theta)} - u\right) H\left(\frac{x}{f'(S^*_R)} - u\right) P_U(u) du \]

\[
= F_{n_{tr}}(\theta; x, t) + \int_{0}^{\infty} \left[ H(\theta - S_{tr}) H\left(\frac{x}{f'(\theta)} - u\right) H\left(\frac{x}{f'(S^*_R)} - u\right) \right] P_U(u) du \]

\[
+ H(\theta - S_D) H\left(\frac{x}{f'(\theta)} - u\right) H\left(\frac{x}{f'(S^*_R)} - u\right) P_U(u) du \tag{C7}
\]

\[
= F_{n_{tr}}(\theta; x, t) + H(\theta - S_{tr}) \left[ F_U\left(\frac{x}{f'(\theta)} - u\right) - F_U\left(\frac{x}{f'(S^*_R)} - u\right) \right] + H(\theta - S_D) \left( 1 - F_U\left(\frac{x}{f'(\theta)} - u\right) \lor \frac{x}{f'(S^*_R)} - u\right) \]

\[
+ H(\theta - S_D) H\left(\frac{x}{f'(\theta)} - u\right) H\left(\frac{x}{f'(S^*_R)} - u\right) P_U(u) du \]

\[
= F_{n_{tr}}(\theta; x, t) + H(\theta - S_{tr}) \left[ F_U\left(\frac{x}{f'(\theta)} - u\right) - F_U\left(\frac{x}{f'(S^*_R)} - u\right) \right] + H(\theta - S_D) \left( 1 - F_U\left(\frac{x}{f'(\theta)} - u\right) \lor \frac{x}{f'(S^*_R)} - u\right) \]

\[
+ H(\theta - S_D) H\left(\frac{x}{f'(\theta)} - u\right) H\left(\frac{x}{f'(S^*_R)} - u\right) P_U(u) du \tag{C7}
\]
Subsequently, for \( x < x_{DP} \), \( S_B < \theta < S_L^* \) the derivation steps are provided in Equation C8. We begin with the third line of Equation 34. Next, we replace the definition of \( \Pi_b \) from Equation 25, III and the definition of the front location for the left-moving wave as \( x_{fl} = f'(S_L^*) U(x,t) \). After a few mathematical manipulations as elaborated for the previous derivations, this expressions lead to the final form of the CDF in the last line, also provided in Equation 37.

\[
F_{s_L}(\theta; x, t) = \int_{0}^{x} \Pi_b H(x - x_{fl}) P_b(u) du \\
= \int_{0}^{x} \left[ H(\theta - S_B) H(C - x) H(x - x_{fl}) + H(\theta - S_B) H(x - C) H(x - x_{fl}) \right] P_b(u) du \\
= H(\theta - S_B) \left[ F_U \left( \frac{x}{f'(S_L^*)} \right) - F_U \left( \frac{x}{f'(\theta)} \right) \right] + H(\theta - S_B) \left[ F_U \left( \frac{x}{f'(\theta)} \wedge \frac{x}{f'(S_L^*)} \right) \right] \\
\] (C8)

Afterward, for \( x < x_{DP}, S_L^* < \theta < S_B \), the derivation steps are provided in Equation C9. We begin with the definition of \( \Pi \) in Equation 22. Next, we replace the definition of the front location \( x_{fl} = f'(S_L^*) U(x,t) \). After a few mathematical manipulations as elaborated for the previous derivations, this expressions lead to the final form of the CDF in the last line, also provided in Equation 38.

\[
F_{s_L}(\theta; x, t) = F_{s_L}(\theta; x, t) + \int_{0}^{x} \Pi_b H(x - x_{fl} - x) P_b(u) du \\
= F_{s_L}(\theta; x, t) + H(S_B - \theta) \int_{0}^{x} H(f'(S_L^*) u - x) P_b(u) du \\
= F_{s_L}(\theta; x, t) + H(S_B - \theta) \int_{0}^{x} \left[ u - \frac{x}{f'(S_L^*)} \right] P_b(u) du \\
= F_{s_L}(\theta; x, t) + H(S_B - \theta) \left[ 1 - F_U \left( \frac{x}{f'(S_L^*)} \right) \right] \\
\] (C9)

It is worth noting that, in this case, we have only combined the CDF of the current range \((S_L^*, S_B)\) with \( F_{s_L}(\theta; x, t) \). We have not combined it with the CDF of the right-moving wave, denoted as \( F_{s_R}(\theta; x, t) \), as the current left-moving wave's range only extends from \([S_B, S_L]\). That is, the movement of the right-moving and left-moving waves, although they start at the same time, are independent from each other.

Finally, for the case of an inverted gravity column, after the waves bounce back from the boundaries (Figure C1), we derive the equations as follows. For \( x < x_{DP}, S_B < \theta < S_L^* \), the derivation steps are provided in Equation C10. We begin with expanding the first line of Equation 39. Next, we replace the definition of \( \Pi_b \) from Equation 25, IV. Then, we substitute the definitions of \( C(\theta, x, t) \) and the front location \( x_{fl} = f'(S_L^*) U(x,t) \). After a few mathematical manipulations as elaborated for the previous derivations, this expressions lead to the final form of the CDF in the last line, also provided in Equation 40.

\[
F_{s_L}(\theta; x, t) = \int_{0}^{x} \Pi_b H \left( x_{fl} - x \right) P_b(u) du \\
= \int_{0}^{x} \left[ H(\theta - S_B) H(x - C) H(x_{fl} - x) + H(\theta - S_B^*) H(C - x) H(x_{fl} - x) \right] P_b(u) du \\
= H(\theta - S_B) \left[ F_U \left( \frac{x}{f'(\theta)} \wedge \frac{x}{f'(S_L^*)} \right) \right] + H(\theta - S_B^*) \left[ 1 - F_U \left( \frac{x}{f'(\theta)} \wedge \frac{x}{f'(S_L^*)} \right) \right] \\
\] (C10)
For $x_{S_L} < x < x_{S_L''}, S_L'' \leq \theta \leq S_{P'},$ the solution is found by aggregating the CDFs of the left wave from earlier times:

$$F_{S_L}(\theta; x, t) = F_{S_L}(\theta; x, t) + F_{S_L}(\theta; x, t)$$

$$= H(\theta - S_B) \left( F_U \left( \frac{x}{f'(S_L')} \right) - F_U \left( \frac{x}{f'(\theta)} \right) \right) + H(\theta - S_D) \left( F_U \left( \frac{x}{f'(\theta)} \wedge \frac{x}{f'(S_L')} \right) \right)$$

$$+ H(\theta - S_a) \left( F_U \left( \frac{x}{f'(\theta)} \right) - F_U \left( \frac{x}{f'(S_L''')} \right) \right) + H(\theta - S_L') \left( 1 - F_U \left( \frac{x}{f'(\theta)} \vee \frac{x}{f'(S_L''')} \right) \right)$$

Additionally, for $x > x_{S_L''}, S_R'' < \theta < 1 - S_w,$ the derivation steps are provided in Equation C12. We begin with expanding the third line of Equation 39. Next, we replace the definition of $\Pi_{b_R}$ from Equation 25, II. Then, we substitute the definitions of $C(\theta, x, t)$ and the front location $x_{S_R} = f'(S_R')U(x, t).$ After a few mathematical manipulations as elaborated in the previous derivations, this expressions lead to the final form of the CDF in the last line, also provided in Equation 43:

$$F_{S_R}(\theta; x, t) = \int_0^\infty \Pi_{b_R} C(x - x_{S_R}^*) P_U(u) du$$

$$= \int_0^\infty \left[ H(\theta - S_B) H(x - C) H(x - x_{S_R}^*) + H(\theta - S_R^*') H(C - x) H(x - x_{S_R}^*) \right] P_U(u) du$$

$$= H(\theta - S_B) \left( F_U \left( \frac{x}{f'(\theta)} \wedge \frac{x}{f'(S_R''')} \right) \right) + H(\theta - S_R^*) \left( F_U \left( \frac{x}{f'(\theta)} \wedge \frac{x}{f'(S_R''')} \right) \right)$$

For $x_{S_R} < x < x_{S_R''}, S_R'' \leq \theta \leq S_R^{**},$ we have:

$$F_{S_R}(\theta; x, t) = F_{S_R}(\theta; x, t) + F_{S_R}(\theta; x, t)$$

$$= F_{S_R}(\theta; x, t)$$

$$+ H(\theta - S_a) \left( F_U \left( \frac{x}{f'(\theta)} \wedge \frac{x}{f'(S_R''')} \right) \right) + H(\theta - S_D) \left( 1 - F_U \left( \frac{x}{f'(\theta)} \vee \frac{x}{f'(S_R'')} \right) \right)$$

$$+ H(\theta - S_B) \left( F_U \left( \frac{x}{f'(\theta)} \wedge \frac{x}{f'(S_R'')} \right) \right) + H(\theta - S_R^*) \left( F_U \left( \frac{x}{f'(\theta)} \wedge \frac{x}{f'(S_R'')} \right) \right)$$

Figure C1. Saturation profile for the inverted gravity column, before and after being reflected from the boundaries. Solid lines are the Monte Carlo solutions of Equation 7, while dashed lines represent the corresponding deterministic solutions.
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References

Baqr, Y., & Chen, X. (2022). A review on reactive transport model and porosity evolution in the porous media. *Environmental Science and Pollution Research*, 29(32), 47873–47901. https://doi.org/10.1007/s11356-022-20466-w

Botv, Z. I., Grotwolski, J. F., & Kroese, D. P. (2010). Kernel density estimation via diffusion. *Annals of Statistics*, 38(5), 2916–2957. https://doi.org/10.1214/aos799

Brenier, Y., & Jaffré, J. (1991). Upstream differencing for multiphase flow in reservoir simulation. *SIAM Journal on Numerical Analysis*, 28(3), 685–696. https://doi.org/10.1137/0728036

Brooks, R. H., & Corey, A. T. (1964). Hydraulic properties of porous media. *Hydrology papers* (Vol. 3). Colorado State University.

Buckley, S. E., & Leverett, M. (1942). Mechanism of fluid displacement in sands. *Transactions of the AIME*, 146(01), 107–116. https://doi.org/10.1109/jcp.2019.01.008

Fan, Y., Durlafsky, L. J., & Tchelepi, H. A. (2012). A fully-coupled flow-reactive-transport formulation based on element conservation, with application to CO2 storage simulations. *Advances in Water Resources*, 42, 47–61. https://doi.org/10.1016/j.advwatres.2012.03.012

Foks, O., Ibrahima, F., Tomin, P., & Tchelepi, H. A. (2019). Analysis of travel-time distributions for uncertainty propagation in channelized porous systems. *Transport in Porous Media*, 126(1), 115–137. https://doi.org/10.1007/s11242-018-1052-z

Gehlen, L. W. (1986). Stochastic subsurface hydrology from theory to applications. *Water Resources Research*, 22(0S), 1355–1455. https://doi.org/10.1029/wr022i09p0135s

Graham, W., & McLaughlin, D. (1989). Stochastic analysis of nonstationary subsurface solute transport: 2. Conditional moments. *Water Resources Research*, 25(11), 2331–2355. https://doi.org/10.1029/WR025i011p02331

Harten, A., Lax, P. D., & Leer, B. V. (1983). On upstream differencing and Godunov-type schemes for hyperbolic conservation laws. *SIAM Review*, 25(1), 35–61. https://doi.org/10.1137/1025002

Ibrahima, F., Meyer, D. W., & Tchelepi, H. A. (2015). Distribution functions of saturation for stochastic nonlinear two-phase flow. *Transport in Porous Media*, 109(1), 81–107. https://doi.org/10.1007/s11242-015-0503-z

Ibrahima, F., & Tchelepi, H. A. (2017). Multipoint distribution of saturation for stochastic two-phase transport. *SIAM/ASA Journal on Uncertainty Quantification*, 5(1), 353–377. https://doi.org/10.1137/16m1096244

Ibrahima, F., Tchelepi, H. A., & Meyer, D. W. (2018). An efficient distribution function method for nonlinear two-phase flow in highly heterogeneous multidimensional stochastic porous media. *Computational Geosciences*, 22(1), 389–412. https://doi.org/10.1007/s10596-017-9698-0

Jarnum, K. D., & Russell, T. F. (2003). Eulerian moment equations for 2-D stochastic immiscible flow. *Multiscale Modeling and Simulation*, 1(4), 598–608. https://doi.org/10.1137/s1540359001343906

Kitanidis, P. K. (1988). Prediction by the method of moments of transport in a heterogeneous formation. *Journal of Hydrology*, 102(1–4), 453–473. https://doi.org/10.1016/0022-1694(88)90111-4

Kwok, P., & Tchelepi, H. A. (2008). Convergence of implicit monotone schemes with applications in multiphase flow in porous media. *SIAM Journal on Numerical Analysis*, 46(5), 2662–2687. https://doi.org/10.1137/070703922

LeVeque, R. J. (2002). *Finite volume methods for hyperbolic problems*. Cambridge University Press.

Li, B., & Tchelepi, H. A. (2015). Nonlinear analysis of multiphase transport in porous media in the presence of viscous, buoyancy, and capillary forces. *Journal of Computational Physics*, 297, 104–131. https://doi.org/10.1016/j.jcp.2015.04.057

Li, B., Tchelepi, H. A., & Benson, S. M. (2013). Influence of capillary-pressure models on CO2 solubility trapping. *Advances in Water Resources*, 62, 488–498. https://doi.org/10.1016/j.advwatres.2013.08.005

Li, H., & Zhang, D. (2007). Probabilistic collocation method for flow in porous media: Comparisons with other stochastic methods. *Water Resources Research*, 43(9), W09409. https://doi.org/10.1029/2006wr005673

Li, H., & Zhang, D. (2009). Efficient and accurate quantification of uncertainty for multiphase flow with the probabilistic collocation method. *SPE Journal*, 14(04), 665–679. https://doi.org/10.2118/114802-pa

Li, L., & Tchelepi, H. A. (2005). Conditional statistical moment equations for dynamic data integration in heterogeneous reservoirs. In SPE Reservoir Simulation Symposium.

Liec, K.-A. (2019). An introduction to reservoir simulation using MATLAB/GNU octave. Cambridge University Press.

Likanapaisal, P., Li, L., & Tchelepi, H. A. (2012). Dynamic data integration and quantification of prediction uncertainty using statistical-moment equations. *SPE Journal*, 17(01), 98–111. https://doi.org/10.2118/119138-pa

Meyer, D. W., Jenny, P., & Tchelepi, H. A. (2010). A joint velocity-concentration PDF method for tracer flow in heterogeneous porous media. *Water Resources Research*, 46(12), W12522. https://doi.org/10.1029/2010wr009450

Meyer, D. W., & Tchelepi, H. A. (2010). Particle-based transport model with Markovian velocity processes for tracer dispersion in highly heterogeneous porous media. *Water Resources Research*, 46(11), W11552. https://doi.org/10.1029/2009wr008925

Meyer, D. W., Tchelepi, H. A., & Jenny, P. (2013). A fast simulation method for uncertainty quantification of subsurface flow and transport. *Water Resources Research*, 49(5), 2359–2379. https://doi.org/10.1002/wrcr.20240

Müller, F., Jenny, P., & Meyer, D. W. (2011). Probabilistic collocation and Lagrangian sampling for advective tracer transport in randomly heterogeneous porous media. *Advances in Water Resources*, 34(12), 1527–1538. https://doi.org/10.1016/j.advwatres.2011.09.005

Müller, F., Jenny, P., & Meyer, D. W. (2013). Multilevel Monte Carlo for two phase flow and Buckley–Leverett transport in random heterogeneous porous media. *Journal of Computational Physics*, 250, 685–702. https://doi.org/10.1016/j.jcp.2013.03.023

Orr, F. M. (2007). *Theory of gas injection processes* (Vol. 5). Tie-Line Publications.

Data Availability Statement

There are no data sharing issues, as all the numerical information is presented in the figures generated through the solution of the equations in the paper.
Pettersson, P., & Tchelepi, H. (2014). Stochastic Galerkin method for the Buckley-Leverett problem in heterogeneous formations. In ECMOR XIV-14th European Conference on the Mathematics of Oil Recovery.

Pope, S. B. (1985). PDF methods for turbulent reactive flows. *Progress in Energy and Combustion Science, 11*(2), 119–192. https://doi.org/10.1016/0360-1285(85)90002-4

Rubin, Y. (2003). *Applied stochastic hydrogeology*. Oxford University Press.

Shalimova, I. A., & Sabelfeld, K. K. (2017). Solution of a stochastic Darcy equation by polynomial chaos expansion. *Numerical Analysis and Applications, 10*(3), 259–271. https://doi.org/10.1134/s1995423917030077

Tchelepi, H. A. (1994). Viscous fingering, gravity segregation and permeability heterogeneity in two-dimensional and three-dimensional flows. Stanford University.

Van Genuchten, M. T. (1980). A closed-form equation for predicting the hydraulic conductivity of unsaturated soils. *Soil Science Society of America Journal, 44*(5), 892–898. https://doi.org/10.2136/sssaj1980.03615995004400050002x

Wang, P., Tartakovsky, D. M., Jarman, K., Jr., & Tartakovsky, A. M. (2013). CDF solutions of Buckley–Leverett equation with uncertain parameters. *Multiscale Modeling and Simulation, 11*(1), 118–133. https://doi.org/10.1137/120865574

Winter, C. L., Tartakovsky, D., & Guadagnini, A. (2003). Moment differential equations for flow in highly heterogeneous porous media. *Surveys in Geophysics, 24*(1), 81–106. https://doi.org/10.1023/a:102227418570

Xiu, D., & Hesthaven, J. S. (2005). High-order collocation methods for differential equations with random inputs. *SIAM Journal on Scientific Computing, 27*(3), 1118–1139. https://doi.org/10.1137/040615201

Yang, H. J., Boso, F., Tchelepi, H. A., & Tartakovsky, D. M. (2019). Probabilistic forecast of single-phase flow in porous media with uncertain properties. *Water Resources Research, 55*(11), 8631–8645. https://doi.org/10.1029/2019wr026090

Yousefzadeh, M. (2020). *Numerical simulation of fluid-mineral interaction and reactive transport in porous and fractured media*. Stanford University.

Zaleski, S., & Panfilov, M. (2017). Model of kinematic waves for gas–liquid segregation with phase transition in porous media. *Journal of Fluid Mechanics, 829*, 659–680. https://doi.org/10.1017/jfm.2017.556

Zhang, D., Li, L., & Tchelepi, H. (2000). Stochastic formulation for uncertainty analysis of two-phase flow in heterogeneous reservoirs. *SPE Journal, 5*(01), 60–70. https://doi.org/10.2118/59802-pa

Zhang, D., & Lu, Z. (2004). An efficient, high-order perturbation approach for flow in random porous media via Karhunen–Loeve and polynomial expansions. *Journal of Computational Physics, 194*(2), 773–794. https://doi.org/10.1016/j.jcp.2003.09.015

Zhang, D., & Tchelepi, H. (1999). Stochastic analysis of immiscible two-phase flow in heterogeneous media. *SPE Journal, 4*(04), 380–388. https://doi.org/10.2118/59250-pa

Zhang, D., & Winter, C. L. (1999). Moment-equation approach to single phase fluid flow in heterogeneous reservoirs. *SPE Journal, 4*(02), 118–127. https://doi.org/10.2118/56842-pa