An Improved Semi-Analytical Solution for Verification of Numerical Models of Two-Phase Flow in Porous Media

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ABSTRACT

A closed-form solution for one-dimensional two-phase flow through a homogeneous porous medium is presented that is applicable to water flow in the vadose zone and flow of nonaqueous phase fluids. The solution is a significant improvement to the one originally presented by McWhorter and Sunada (1990), allowing the analysis of wetting phase entry saturations ranging from residual to full. Our aims are to provide a detailed analysis of how the solution to the governing partial differential equation of two-phase flow can be obtained from a functional integral equation arising from the analytical treatment of the problems and to present an improved algorithm for the implementation of this solution. The integral functional equation is obtained by imposing a set of assumptions for the boundary conditions. The proposed method can be used to obtain solutions that incorporate a wide range of saturation values at the entry point. The semi-analytical solution will be useful in the verification of vadose zone flow and multi-phase flow codes designed to simulate more complex two-phase flow problems in porous media where capillary effects must be included.

Keywords

Benchmarks for two-phase flow; vadose zone code verification; Buckley-Leverett equation; capillarity and advection;

1. Introduction

Complex multi-dimensional numerical models of multi-phase flow through porous media such as those described by Helmig (1997), Mikyška et al. (2004), or Mikyška and Illangasekare (2005) require verification to assure that the governing equations are solved correctly and the codes do not contain programming errors. This step of code verification is a necessary step in modeling protocols used in practice (e.g., Anderson & Woessner (2002)). Code simulations are compared to closed-form analytical solutions of the governing equations to estimate numerical errors and other inaccuracies of numerical schemes. Two well-known one-dimensional solutions of the two-phase flow equations include the Buckley-Leverett solution of flow without capillary effects (e.g., described by Helmig (1997) and LeVeque (2002); or see references in McWhorter and Sunada (1990)), and the exact integral solution derived by McWhorter and Sunada (1990) with subsequent discussions by Chen et al. (1992), McWhorter and Sunada (1992), and Fučík et al. (2005), which includes both advective and capillary effects. In this paper, we discuss the exact integral equation for the wetting-phase saturation obtained by McWhorter and Sunada (1990). This equation must be numerically integrated to yield the saturation distribution along the length of the soil column, and a value

for entry saturation is needed as an input boundary condition. The solution to the problem as presented by McWhorter and Sunada (1990) has limitations in those situations where the entry wetting-phase saturations are high.
As numerical models are designed to simulate conditions that include high entry wetting saturations (e.g., wetting front propagation, water flooding for enhanced recovery), analytical models used for code verification should have the capability to simulate this flow condition. We present an improvement of the technique, that allows the exact integral solution to be reliably obtained under conditions where the McWhorter and Sunada (1990) approach fails to converge. Our approach provides insight into the solution behavior and explains the limitations of the previously known method of resolution of the integral equation. This generalized approach is applicable to unsaturated zone (water - air) or saturated zone (water - NAPL) models when both phases are assumed to be incompressible. We perform a series of qualitative and quantitative computations that show our algorithm agrees with previously obtained results while demonstrating the improved performance.

2. Two-phase flow model

In this section we introduce basic notation and set up the governing equations.

2.1 Transport equation with capillarity

We consider a one-dimensional problem describing flow of two incompressible and immiscible fluids through a porous medium where the non-wetting phase (indexed n) is horizontally displaced by the wetting fluid (water, indexed w) (therefore neglecting the influence of gravity). Darcy's law, when written for each of the fluid phases, has the following form:

$$q_\alpha = -\lambda_\alpha \frac{\partial p_\alpha}{\partial x}, \tag{1}$$

where q_α, λ_α, and p_α are the flux, mobility and pressure of the phase α, respectively, where we use $\alpha \in \{w, n\}$. The α-phase mobility is defined as

$$\lambda_\alpha = \frac{k_\alpha}{\mu_\alpha}, \tag{2}$$

where k_α is the permeability and μ_α is the dynamic viscosity of phase α (Bastian, 1999). The total flux q_t is defined as the sum of the fluxes of each of the phases $(q_t = q_w + q_n)$. The capillary relation, $p_c = p_n - p_w$, with a given function $p_c = p_c(S_w)$ of the effective wetting phase saturation S_w, links the wetting and the nonwetting balance equations. The effective saturation of the phase α is defined by

$$S_\alpha = \frac{s_\alpha - S_{\alpha r}}{1 - S_{wr} - S_{nr}}, \tag{3}$$

where S_{wr} and S_{nr} are the residual wetting and non-wetting phase saturations, respectively, and s_α is the saturation of phase α. The effective saturation is always between 0 and 1, which simplifies the description of the dependent variable by the definition $S_w + S_n = 1$ (Helmig, 1997).
Introducing the wetting and nonwetting phase fractional flow functions

$$f_\alpha(S_w) = \frac{\lambda_\alpha(S_w)}{\lambda_w(S_w) + \lambda_n(S_w)}, \tag{4}$$

and diffusivity functions

$$D_w(S_w) = -\frac{\lambda_w(S_w)\lambda_n(S_w)}{\lambda_w(S_w)+\lambda_n(S_w)}\frac{dp_c(S_w)}{dS_w}, \tag{5}$$

$$D_n(S_w) = \frac{\lambda_w(S_w)\lambda_n(S_w)}{\lambda_w(S_w)+\lambda_n(S_w)}\frac{dp_c(S_w)}{dS_w}, \tag{6}$$

we obtain the expression for the α -phase flux as

$$q_\alpha = f_\alpha(S_w)\, q_t - D_\alpha(S_w)\frac{\partial S_w}{\partial x}. \tag{7}$$

The mass-balance equation has the following form (the fluid mass density is assumed constant):

$$\frac{\partial q_\alpha}{\partial x} + \Phi(1-S_{wr}-S_{nr})\frac{\partial S_\alpha}{\partial t} = 0, \tag{8}$$

where Φ is the porosity.

The two-phase flow equation is obtained by substituting (7) into the mass-balance equation (8) to yield

$$\Phi(1-S_{wr}-S_{nr})\frac{\partial S_w}{\partial t} = -q_t\frac{\partial f_w(S_w)}{\partial x} + \frac{\partial}{\partial x}\left(D_w(S_w)\frac{\partial S_w}{\partial x}\right), \tag{9}$$

which corresponds to equation (2) in McWhorter and Sunada (1990). Substituting $S_w = 1 - S_n$, equation (9) becomes

$$\Phi(1-S_{wr}-S_{nr})\frac{\partial S_n}{\partial t} = -q_t\frac{\partial f_n(1-S_n)}{\partial x} + \frac{\partial}{\partial x}\left(D_n(1-S_n)\frac{\partial S_n}{\partial x}\right). \tag{10}$$

Equations (9) and (10) are equivalent and they can be used in the formulation of either a wetting phase or a nonwetting phase displacement problem. A general form of the two-phase flow equation is given as

$$\Phi(1-S_{wr}-S_{nr})\frac{\partial S}{\partial t} = -q_t\frac{\partial f(S)}{\partial x} + \frac{\partial}{\partial x}\left(D(S)\frac{\partial S}{\partial x}\right), \tag{11}$$

where we obtain equations (9) or (10) using respective substitutions for the functions f, D and S. For the one-dimensional displacement problem, the initial and boundary saturations (at $x = 0$ and $x \to +\infty$) must be defined.

McWhorter and Sunada (1990) presented the closed-form analytical solution for equation (11) for both one-dimensional and radial displacement. The radial displacement problem presented in McWhorter and Sunada (1990) is not discussed in this paper because a different type of the integral equation arises in that case.

We will discuss conditions under which the flow equation can be solved analytically to provide a simple one-dimensional benchmark solution for verification of more complex two-phase flow codes.

2.2 Transport equation without capillarity

The last term in equation (11) vanishes when the capillary effects represented by the term $dp_c(S)/dS$ in the diffusivity function $D(S)$ are neglected, resulting in the Buckley-Leverett equation for two-phase flow (Helmig, 1997)

$$\Phi(1-S_{wr}-S_{nr})\frac{\partial S}{\partial t} = -q_t\frac{df(S)}{dS}\frac{\partial S}{\partial x}. \tag{12}$$

The first-order hyperbolic equation (12) represents a limiting case for equation (11) when $D(S) \to 0$. The boundary and initial conditions are defined as

$$S(0,x)=S_i,$$
$$S(t,0)=S_0.$$

The analytical solution to equation (11) is based on the method of characteristics and is given by

$$x(t,S)=\frac{1}{\Phi(1-S_{wr}-S_{nr})}\frac{df_w(S)}{dS}\int_0^t q_t(\tau)d\tau. \tag{13}$$

The function $f(S)$ has an inflection point, so that the solution is implicitly given by equation (13) for $S_0 \geq S \geq S_t$ (inverted saturation profile), where S_t is the Welge tangent saturation (or post-shock value; see LeVeque (2002)) that is determined from the relation

$$\frac{df_w(S_t)}{dS}=\frac{f_w(S_t)-f_w(S_i)}{S_t-S_i}. \tag{14}$$

2.3 Capillary and relative-permeability model functions

Denoting the intrinsic permeability of the medium by k, the relative permeability for the wetting phase is defined by $k_{rw}=k_w/k$ and the relative permeability for the nonwetting phase by $k_{rn}=k_n/k$. The functions k_{rw}, k_{rn} and the capillary-pressure expression are used in the following formulations.

The Brooks-Corey model (Brooks and Corey, 1964) relating capillary pressure p_c to saturation is given by

$$p_c(S)=P_0\, S^{-\frac{1}{\lambda}}, \tag{15}$$

where λ and P_0 are parameters characterising the soil and phase properties; P_0 is called the *entry pressure*.

Application of the Burdine (1953) formulation to the Brooks-Corey model results in relative permeability functions for the wetting and non-wetting phases in the form

$$k_{rw}(S)=S^{3+\frac{2}{\lambda}}, \tag{16}$$
$$k_{rn}(S)=(1-S)^2(1-S^{1+\frac{2}{\lambda}}).$$

The van Genuchten (1980) capillary-pressure p_c expression is given as

$$p_c(S)=P_0\left(S^{-\frac{1}{m}}-1\right)^{\frac{1}{n}}, \tag{17}$$

where the parameters m and n are often related by $m=1-\frac{1}{n}$.

Application of the Mualem (1976) relative-permeability functions to the van Genuchten model results in

$$k_{rw}(S)=S^{\frac{1}{2}}\left(1-(1-S^{\frac{1}{m}})^m\right)^2, \tag{18}$$
$$k_{rn}(S)=(1-S)^{\frac{1}{3}}\,(1-S^{\frac{1}{m}})^{2m}.$$

3. Quasi-analytical solution

Usefulness of a benchmark solution depends on its relative ease of use. We therefore consider the possibility of improving a closed-form solution to equation (11) based on the approach originally presented by McWhorter and Sunada (1990). In this section, The closed-form solution of McWhorter and Sunada (1990) is presented in this section to provide a basis for improvement. An enhancement that enables a wider range of entry saturations to be considered than the McWhorter and Sunada (1990) approach is presented in Section 4.

3.1 Problem formulation

A quasi-stationary solution of (11) under a particular set of conditions is presented. We assume that for all $x \in (0, +\infty)$ and $t \in [0, +\infty)$

$$S(t,0) = S_0, \tag{19}$$

$$S(t,+\infty) = S_i, \tag{20}$$

$$S(0,x) = S_i, \tag{21}$$

with $S_0 > S_i$. If $S_0 < S_i$, we must use the other formulation (i.e., (10) instead of (9)) or introduce a fractional flow function, F_{nw}, as in McWhorter and Sunada (1990). An advantage of our approach is that we use the same code to compute the wetting as well as the non-wetting phase displacement problem simply by defining respective functions f and D appropriately.

The displacing phase (indexed α) is introduced to the column at $x = 0$ with volumetric flux given by

$$q_\alpha(t,0) = A\,g(t) = A\,t^{-\frac{1}{2}}, \tag{22}$$

where $A > 0$. The function $g(t)$ must have the form $g(t) = t^{-\frac{1}{2}}$, as will be shown in Section 3.4. The displaced phase flux at the inlet ($x = 0$) and the outlet ($x \to +\infty$) are unknown. The boundary at $x \to +\infty$ is semi-permeable, characterized by a scalar coefficient $R \in [0,1]$, where $R = 0$ implies that the boundary is impermeable and $R = 1$ implies no resistance to the flow at the boundary (unidirectional flow).

It follows from (7) and from the assumption of incompressibility of both phases that

$$\frac{\partial q_t}{\partial x} = 0. \tag{23}$$

Therefore, q_t is spatially uniform but may vary with time, i.e., for all $x \geq 0$ and $t \geq 0$ we get

$$q_t(t,x) = R\,q_\alpha(t,0) = RAg(t). \tag{24}$$

The total flux achieves its maximum value, $q_t(t) = Ag(t)$, at the outlet when $R = 1$. On the other hand, the total flux vanishes when $R = 0$. This represents bidirectional displacement where the displaced fluid is draining only at the inlet ($x = 0$).

McWhorter and Sunada (1990) considered only the limiting cases of $R = 0$ and $R = 1$, but we note that the approach is valid for $R \in [0,1]$. The displacing phase is thus injected in the counter-current flow direction of the total flux q_t.

By combining equations (7), (22), and (24), we obtain the relationship

$$\frac{\partial S}{\partial x}(t,0) = -A\,g(t)\,\frac{1 - R\,f(S_0)}{D(S_0)}. \tag{25}$$

3.2 Basic assumptions

We assume that the solution exists in the form $S = S(\lambda)$, where

$$\lambda = x\,g(t). \tag{26}$$

This substitution is possible, provided the *basic assumption*

$$S = S(\lambda) \text{ is a strictly monotone function of } \lambda. \tag{27}$$

This assumption allows the dependence $S = S(\lambda)$ to be inverted so that $\lambda = \lambda(S)$.

Assuming that S as a function of λ is sufficiently smooth, partial differentiation of (26) yields

$$\frac{\partial S}{\partial t}(t,x) = \frac{\lambda[S(t,x)]}{\lambda'[S(t,x)]}\frac{g'(t)}{g(t)} \ , \tag{28}$$

and

$$\frac{\partial S}{\partial x}(t,x) = \frac{g(t)}{\lambda'[S(t,x)]} \ , \tag{29}$$

where $g'(t)$ and $\lambda'(S)$ stand for the derivatives $dg(t)/dt$ and $d\lambda(S)/dS$, respectively.

3.3 Expression for Function F

We define the fractional flow function, $F = F(t,x)$, as

$$F(t,x) = R\frac{f[S(t,x)] - f(S_i)}{1 - R\ f(S_i)} - \frac{D[S(t,x)]}{Ag(t)\,(1 - R\ f(S_i))}\frac{\partial S}{\partial x}(t,x), \tag{30}$$

and introduce the normalized fractional flow function, $\varphi(S)$, where

$$\varphi(S) = R\frac{f(S) - f(S_i)}{1 - R\ f(S_i)}. \tag{31}$$

Combining equations (29), (30) and (31) allows for the redefinition of F in terms of S,

$$F(S) = \varphi(S) - \frac{1}{A(1 - R\ f(S_i))}\frac{D(S)}{\lambda'(S)}. \tag{32}$$

3.4 Stationary differential equation

Introduction of expression (32) for F to equation (11) yields

$$\Phi(1 - S_{wr} - S_{nr})\frac{\partial S}{\partial t} + Ag(t)\,(1 - R\ f(S_i))\frac{\partial F(S)}{\partial x} = 0. \tag{33}$$

Substituting equation (26), (28), and (29) into (33), we obtain the equation

$$\Phi(1 - S_{wr} - S_{nr})\frac{g'(t)}{g^3(t)}\lambda(S) + A(1 - R\ f(S_i))F'(S) = 0, \tag{34}$$

where $F'(S)$ stands for $dF(S)/dS$.

Only a function g of the form

$$g(t) = (-2\,C_1\,t + C_2)^{-\frac{1}{2}} \tag{35}$$

allows the removal of the explicit time dependence of the terms in equation (34) because the term $g'(t)/g^3(t)$ equals C_1. The value of C_1 is arbitrary as long as it is negative. As the value of A depends on C_1, it is therefore possible to choose for instance $C_1 = -1/2$.

Differentiating (34) with respect to S and substituting equation (32) for $F(S)$ yields the second-order ordinary differential equation

$$F''(S) = -\frac{\Phi(1 - S_{wr} - S_{nr})}{2A^2(1 - R\ f(S_i))^2}\frac{D(S)}{F(S) - \varphi(S)}, \tag{36}$$

where $F''(S)$ stands for $d^2F(S)/dS^2$.

The boundary conditions for the ordinary differential equation (36) are $F(S_0)=1$ and $F(S_i)=0$, which follow from (19) and (21), respectively. Note that matching the initial condition (21) to the condition $F(S_i)=0$ is possible only if $g(0)=+\infty$. This implies that the only possible form of the input flux function $g(t)$ is $g(t)=t^{-\frac{1}{2}}$, which in turn implies that $C_2=0$ by (35).

Moreover, the boundary condition defined in (19) gives us $F'(S_0)=0$. However, the problem is not overdetermined because the condition $F(S_i)=0$ will be used to establish the relationship between A and S_0.

3.5 Solution of the transport equation

Once the function $F(S)$ is known, we can derive the inverted form of (11) from the relation

$$\frac{2A(1-R\ f(S_i))}{\Phi(1-S_{wr}-S_{nr})}F'(S)=\lambda(S)=x(t,S)\ g(t), \tag{37}$$

which is in a form similar to the Buckley-Leverett analytical solution (13), given by

$$x(t,S)=\frac{1-R\ f(S_i)}{\Phi(1-S_{wr}-S_{nr})}\frac{dF(S)}{dS}\int_0^t Ag(\tau)d\tau. \tag{38}$$

This expression is valid for all values of $S\in[S_i,S_0]$ because the function $dF(S)/dS$ can be inverted as a consequence of the basic assumption expressed in (27).

In order to demonstrate the relationship between the Buckley-Leverett and the McWhorter-Sunada exact solutions, we define the Buckley-Leverett fractional flow function F_{BL} as follows:

$$F_{BL}=\begin{cases}\varphi(S) & \forall S\geq S_t\\ \varphi(S_t)\dfrac{S-S_i}{S_t-S_i} & \forall S<S_t\end{cases}, \tag{39}$$

where S_t is the Welge tangent saturation given by (14). It is obvious that the function F_{BL} does not satisfy the basic assumption (27) due to the relationship (37) and the linear part of F_{BL}. However, the solutions (13) and (38) are formally the same when F_{BL} is substituted for F.

4. Integral solution

4.1 Derivation

The equation (36) cannot be solved until the relationship between A and S_0 is determined. Following McWhorter and Sunada (1990), we integrate (36) twice and include $F'(S_0)=0$ and $F(S_0)=1$ to obtain

$$F(S)=1-\frac{\Phi(1-S_{wr}-S_{nr})}{2A^2(1-Rf(S_i))^2}\int_S^{S_0}\frac{(v-S)\ D(v)}{F(v)-\varphi(v)}dv. \tag{40}$$

The condition $F(S_i)=0$ allows for the establishment of the relationship between A and S_0 as follows

$$A^2 = \frac{\Phi(1-S_{wr}-S_{nr})}{2(1-Rf(S_i))^2} \int_{S_i}^{S_0} \frac{(v-S_i)\,D(v)}{F(v)-\varphi(v)}\,dv. \tag{41}$$

The integral equation (40) can be rewritten by means of (41) into the form

$$F(S) = 1 - \frac{\int_S^{S_0} \frac{(v-S)\,D(v)}{F(v)-\varphi(v)}\,dv}{\int_{S_i}^{S_0} \frac{(v-S_i)\,D(v)}{F(v)-\varphi(v)}\,dv}. \tag{42}$$

Differentiating this integral equation, we obtain the function $F'(S)$

$$F'(S) = \frac{\int_S^{S_0} \frac{D(v)}{F(v)-\varphi(v)}\,dv}{\int_{S_i}^{S_0} \frac{(v-S_i)\,D(v)}{F(v)-\varphi(v)}\,dv}. \tag{43}$$

The magnitude of the *diffusion term* $D(S)$ does not influence the function F because multiplicative constants in the term $D(S)$ can be cancelled in (42) as well as in (43). It affects only the value of A in (41).

4.2 Iteration scheme

In agreement with McWhorter and Sunada (1990), the unknown function $F(S)$ is computed from the integral equation (42) by iteration. The iterative process is as follows:

$$F_{k+1}(S) = 1 - \frac{\int_S^{S_0} \frac{(v-S)\,D(v)}{F_k(v)-\varphi(v)}\,dv}{\int_{S_i}^{S_0} \frac{(v-S_i)\,D(v)}{F_k(v)-\varphi(v)}\,dv}. \tag{44}$$

As in McWhorter and Sunada (1990), we suggest using $F_0 \equiv 1$ as a first guess. The function F_k is considered to be the solution of (40) when successive iterations are sufficiently small in a norm. In our case, we use the L_∞ norm and terminate the iterative process when

$$\left\| F_k - F_{k+1} \right\|_{L_\infty} < \varepsilon_F. \tag{45}$$

The integrals in (44) are evaluated numerically, therefore the exact solution is often referred to as *quasi-analytical* solution. The iterative process is rapid and convergent for all values of S_0 in case of the bidirectional flow ($R = 0$). However, serious difficulties occur when S_0 and R are close to one as the following first-iteration analysis demonstrates.

4.3 Test problems

Table 1 gives the parameter values that are used to demonstrate our approach. Water is the wetting phase in our computational experiments, while various realistic or theoretical non-wetting liquids are used. The term NAPL stands for non-aqueous phase liquid and DNAPL is denser-than-water NAPL.

The first setup consists of the use of Brooks-Corey model functions and artificially selected values of the soil parameters (see Helmig (1997)). In Setup 1, we choose $\mu_n = 0.020$. Note that efficiency of our approach increases with decreasing μ_w/μ_n.

Setups 2 and 3 contain the parameters of laboratory test soils used in our ongoing research (sand #30 as in Turner (2004), p.43) and a test NAPL Soltrol 220.

	Par.	Units	Setup 1	Setup 2	Setup 3
Porosity	Φ	$[-]$	0.3	0.4	
Intrinsic Permeability	k	$[m^2]$	10^{-10}	$2.26 \cdot 10^{-10}$	
Residual Water Sat.	S_{wr}	$[-]$	0	0.144	
Residual NAPL Sat.	S_{nr}	$[-]$	0	0.069	
Water Viscosity	μ_w	$[kg\ m^{-1}s^{-1}]$	0.001	0.001	
DNAPL Viscosity	μ_n	$[kg\ m^{-1}s^{-1}]$	0.020	0.0035 (Soltrol 220)	
Model functions			Brooks-Corey	Brooks-Corey	van Genuchten
	P_0	$[Pa]$	1000	668	909
	λ	[-]	2	2.29	
	m	[-]			0.75

Table 1. Parameter values for the soil and liquids used in the computational examples.

4.4 First iteration

The iterative scheme presented by McWhorter and Sunada (1990) exhibits unsatisfactory behavior when the denominator in the integrand $D(v)/(F(v)-\varphi(v))$ in (42) approaches zero. This happens when both S_0 and R are close to 1. We offer an analytical justification of this phenomenon. It can be shown that $F(S) > \varphi(S)$ for all $S \in (S_i, S_0)$. Hence, this relationship must stand for all approximations F_k of the function F.

The first iteration of the function F is obtained by substituting $F_0 \equiv 1$ into the right hand side of integral equation (44). Using Brooks-Corey model functions (16) and (15), the first iteration F_1 for the S_w formulation is expressed analytically as follows:

$$F_1(S_w) = 1 - \frac{S_0^{3+\frac{1}{\lambda}}(3\lambda S_0 - 4\lambda S_w - S_w) + \lambda S_w^{4+\frac{1}{\lambda}}}{S_0^{3+\frac{1}{\lambda}}(3\lambda S_0 - 4\lambda S_i - S_i) + \lambda S_i^{4+\frac{1}{\lambda}}}. \tag{46}$$

The second iteration of the function F cannot be computed by substituting F_1 into the right hand side of integral equation (44) for certain values of S_0, because the function F_1 intersects the function φ and the integrand $D(v)/(F(v)-(v))$ becomes unbounded. This is illustrated in Figure 1, where we set $S_i = 0$, $R = 1$ and $S_0 \in \{0.5, 0.7, 0.9, 1\}$.

Equation (46) implies that the first iteration of F is only dependent on λ. We studied the behavior of F_1 with respect to φ for common values of λ, finding that λ does not affect the formation of the instability of the iterative process in any remarkable way.

Although the values μ_w and μ_n do not influence F_1, they have an important impact on the instability formation of the iterative process by the function φ, as shown in Figure 1. As an illustration we study the non-wetting phase displacement problem with $R = 1$ and $S_i = 0$, i.e. $\varphi \equiv f_w$. Whenever the function φ intersects the first iteration F_1, a singularity in the integrand $D(v)/(F(v)-\varphi(v))$ in (42) occurs.

The *viscosity ratio,* $M = \mu_w/\mu_n$, is the key parameter that affects the stability of the iterative process because it shifts the inflexion point of the function φ towards S_0 or S_i (see Figure

1). The singularity may occur at any saturation in the interval (S_i, S_0), not just in the vicinity of S_0. The other parameter that influences the formation of the instability after the first iteration is the initial saturation, S_i, which appears in both the function φ and F_1.

S_i	Viscosity ratio μ_w/μ_w				
	0.001	0.01	1	100	1000
0.00	0.33593	0.52734	0.91578	0.99728	0.99984
0.10	0.30390	0.49330	0.90798	0.99824	0.99976
0.20	0.30468	0.45937	0.89843	0.99656	0.99966
0.30	0.41142	0.45790	0.88378	0.99602	0.99957
0.40	0.52743	0.54003	0.86640	0.99527	0.99970
0.50	0.63696	0.64037	0.84570	0.99413	0.99928
0.60	0.73642	0.73730	0.82968	0.99230	0.99896
0.70	0.82395	0.82414	0.84648	0.98904	0.99842
0.80	0.89818	0.89821	0.90151	0.98261	0.99843

Table 2. Critical values S_0^* for Setup 1.

In displacement problems involving NAPLs that are less viscous than water, as is demonstrated in Tables 2, 3 and 4, the original iterative process fails for values of S_0 near 1 . In order to demonstrate limits of the functionality of the original iterative scheme, we introduce the *critical value* denoted by S_0^* that represents the lowest value of S_0 for which the original iterative scheme (44) fails after the first iteration. We determine S_0^* experimentally by bisectioning an interval $[S_0^{(1)}, S_0^{(2)}]$, where $S_0^{(1)}$ and $S_0^{(2)}$ corresponds to S_0 for which the iterative scheme (44) is stable and fails, respectively. In the next step, we test if the scheme (44) works for $S_0^{(3)} = (S_0^{(1)} + S_0^{(2)})/2$ and then we shift the left ($S_0^{(1)} := S_0^{(3)}$) or the right ($S_0^{(2)} := S_0^{(3)}$) boundary of the interval, so that the scheme (44) works for $S_0 = S_0^{(1)}$ and fails for $S_0 = S_0^{(2)}$. Iterations are terminated when the length of the interval $[S_0^{(1)}, S_0^{(2)}]$ is below a prescribed tolerance.

S_i	Viscosity ratio μ_w/μ_w				
	0.001	0.01	1	100	1000
0.00	0.32018	0.51366	0.91241	0.99715	0.99982
0.10	0.30390	0.47880	0.90463	0.99824	0.99973
0.20	0.30312	0.44335	0.89335	0.99641	0.99980
0.30	0.41347	0.45295	0.87831	0.99584	0.99954
0.40	0.52946	0.54032	0.85929	0.99503	0.99970
0.50	0.63889	0.64208	0.83886	0.99384	0.99920
0.60	0.73798	0.73886	0.82460	0.99191	0.99890
0.70	0.82500	0.82520	0.84648	0.98849	0.99832
0.80	0.89872	0.89877	0.90195	0.98281	0.99843

Table 3. Critical values S_0^* for Setup 2.

Results given in Tables 2, 3, and 4 suggest that the instability issue of the original process is not peripheral for highly viscous non-wetting fluids. For example, the original iterative process fails for values of S_0 greater than 0.82 in the case of the test NAPL Soltrol 220 (Setup 2, Table 1), which is more viscous than water, $\mu_n = 0.0035\, kg\ m^{-1}\ s^{-1}$, so that $M = 0.286$.

Based on Figure 1, the original iterative process will fail for the values of $S_0 \geq S_0^*$.

S_i	Viscosity ratio μ_w/μ_w				
	0.001	0.01	1	100	1000
0.00	0.27734	0.52319	0.98449	0.99998	0.99999
0.10	0.23359	0.47792	0.98143	0.99998	0.99999
0.20	0.32031	0.44921	0.97714	0.99997	0.99999
0.30	0.44731	0.49277	0.97163	0.99996	0.99999
0.40	0.56977	0.58690	0.96410	0.99995	0.99999
0.50	0.68108	0.68798	0.95483	0.99993	0.99999
0.60	0.77875	0.78123	0.94492	0.99991	0.99999
0.70	0.86109	0.86193	0.93784	0.99988	0.99999
0.80	0.92667	0.92687	0.94645	0.99982	0.99999

Table 4. Critical values S_0^* for Setup 3.

4.5 Modified integral equation

We propose the following modified method to avoid unstable behaviour of the numerical iterative process. Denoting the principal part of the integrand in (42) as $G = D/(F-\varphi)$, we can rewrite equation (42) as

$$F(S) = \frac{D(S)}{G(S)} + \varphi(S) = 1 - \frac{\int_S^{S_0} (v-S)G(v)\,dv}{\int_{S_i}^{S_0} (v-S_i)G(v)\,dv}, \tag{47}$$

which allows us to deduce two types of iterative schemes; *method A*, given by the scheme

$$G_{k+1}(S) = D(S) + G_k(S)\left(\varphi(S) + \frac{\int_S^{S_0} (v-S)\,G_k(v)\,dv}{\int_{S_i}^{S_0} (v-S_i)\,G_k(v)\,dv} \right), \tag{48}$$

and *method B*, given by the scheme

$$G_{k+1}(S) = \left[D(S) + G_k(S)\,\varphi(S) \right] \left(1 - \frac{\int_S^{S_0} (v-S)\,G_k(v)\,dv}{\int_{S_i}^{S_0} (v-S_i)\,G_k(v)\,dv} \right)^{-1}. \tag{49}$$

We suggest using $G_0 = D/(1-\varphi)$ as the initial guess, which is equivalent to the case where $F_0 \equiv 1$, as proposed by McWhorter and Sunada (1990).

The integrals in (48) and (49) are evaluated numerically, taking advantage of the form of the integrand as follows. Let $\{G^j\}_{j=0}^{M}$ be an equidistant discretization of the function G in the interval $[S_i, S_0]$, defined as $G^j = G(S_i + j\,h)$, where $h = (S_0 - S_i)/M$. The numerical solution of the integral equations (48) and (49) requires computation of the integral

$$\int_{S}^{S_0} (v-S)\, G_k(v)\, dv. \tag{50}$$

We suggest introducing partial numerical integrals a^j and b^j, given as

$$\underbrace{\int_{S_i+j\,h}^{S_i+(j+1)h} vG(v)\, dv}_{a^j} - S \underbrace{\int_{S_i+j\,h}^{S_i+(j+1)h} G(v)\, dv}_{b^j}. \tag{51}$$

Linear interpolation of $\{G^j\}_{j=0}^{M}$ in the interval $[S_i, S_0]$ allows the value of a^j and b^j to be expressed as

$$a^j = \frac{h}{2} S_i (G^j + G^{j+1}) + \frac{h^2}{6}((3j+1)G^j + (3j+2)G^{j+1}), \tag{52}$$

and

$$b^j = \frac{h}{2}(G^j + G^{j+1}). \tag{53}$$

The integral (50) in the modified iterative schemes (48) and (49) is approximated by I^l for discrete values of saturation ($S = S_i + l\,h$) by

$$\int_{S_i+l\,h}^{S_0} (v - S_i - l\,h)\, G(v)\, dv \approx I^l \overset{def}{=} \sum_{j=l}^{M-1} a^j - (S_i + l\,h) \sum_{j=l}^{M-1} b^j. \tag{54}$$

Since both $F(S_i) = 0$ and $\varphi(S_i) = 0$ by definition, it follows from $G = D/(F-\varphi)$ that the value of $G(S_i)$ is undefined (note that $D(S_i) > 0$ if $S_i > 0$). The value $G_k^0 = G(S_i) = 0$ is used in the scheme for all k.

Application of the discretization $D^l = D(S_i + l\,h)$ and $\varphi^l = \varphi(S_i + l\,h)$ and using the expression (54) in the method A (48) yields

$$G_{k+1}^l = D^l + G_k^l \left(\varphi^l + \frac{I^l}{I^0} \right), \quad \text{where} \quad l = 1, 2, \ldots, M. \tag{55}$$

Analogously, the method B (49) is given by the scheme

$$G_{k+1}^l = \left[D^l + G_k^l\, \varphi^l \right] \left(1 - \frac{I^l}{I^0} \right)^{-1}, \quad \text{where} \quad l = 1, 2, \ldots, M. \tag{56}$$

The presented form of the iterative scheme benefits from the type of the integral equations (42), (48) and (49). In all iterations, only M numbers a^j and b^j need to be evaluated.

Values of the functions F_k are computed from

$$F^l = \frac{D^l}{G^l} + \varphi^l, \tag{57}$$

as $G(S) > 0$ for all $S \in (S_i, S_0)$. It is better to determine the first derivative F' based on the expression (43) in the form

$$F'(S_i + l\,h) = \frac{1}{I^0}\sum_{j=l}^{M-1} b^j \tag{58}$$

than using the numerical differentiation since the terms a^j and I^0 are already evaluated.

4.6 Behavior of the modified iterative scheme

In this section we focus on the unidirectional case with $R = 1$ and will illustrate the functionality of the modified method. We observe a monotone growth of successive estimates of G in all computations, i.e. $G_k \le G_{k+1}$ in $[S_i, S_0]$, and fast convergence for all cases where the original iterative method succeeds (Table 5).

Case	S_0							
	0.4	0.5	0.6	0.7	0.8	0.9	0.99	0.999
Setup 1 with $S_i = 0$								
Original equation (44)	13	12	18	failed	failed	failed	failed	failed
Method A (48)	574	628	637	1645	8342	89684	75356132	$>10^9$
Method B (49)	36	115	411	1645	8348	89681	75459253	$>10^9$
Setup 2 with $S_i = 0$								
Original equation (44)	13	13	13	14	27	failed	failed	failed
Method A (48)	636	711	772	807	1655	17913	15570965	$>10^9$
Method B (49)	29	31	87	320	1652	17925	15595550	$>10^9$
Setup 3 with $S_i = 0$								
Original equation (44)	14	14	14	14	15	27	failed	failed
Method A (48)	1527	1747	1937	2103	2198	2027	121888	7062455
Method B (49)	36	38	46	99	294	1493	121891	7067090
Setup 2 with $S_i = 0.2$								
Original equation (44)	20	19	18	18	failed	failed	failed	failed
Method A (48)	38	25199	29088	32236	31501	17723	15368374	$>10^9$
Method B (49)	7	136	88	323	1654	failed	15345177	$>10^9$
Setup 3 with $S_i = 0.2$								
Original equation (44)	22	21	20	19	19	46	failed	failed
Method A (48)	20523	24836	29106	33519	38123	40250	119475	6836971
Method B (49)	630	157	failed	68	292	1477	119467	failed

Table 5. Number of iterations required to obtain the function F and the value of A with accuracy $\varepsilon_A = 10^{-15}$. In some situations with $S_i > 0$, the modified iterative method B fails randomly.

The modified method converged for cases where the original method failed. In the modified method, successive estimates of G decreased in the L_∞ norm, but the number of iterations needed to reach a required precision of G increases considerably as both S_0 and R approach one. Although there are negligible variations in successive estimates F_k in this situation, the value of A converges slowly, as shown in Figure 2. Successive differences of the function F estimates decrease very rapidly in the beginning of the iterative process, while the value of A increases considerably. Values of ε_F between 10^{-20} to 10^{-35} are necessary to obtain successive differences of the approximations of A below $\varepsilon_A = 10^{-15}$, which reaches the common computer round-off error.

We suggest using the difference between successive approximations of A as the stopping criterion for the iterative process. This is represented formally as

$$\|A_k - A_{k+1}\| < \varepsilon_A. \tag{59}$$

We use the test models with highly viscous NAPL to demonstrate robustness of our modified iterative scheme in situations where the original iterative scheme fails even after the first iteration.

We found that the method B (49) fails randomly due to numerical division by zero, when $S_i > 0$, because finite-precision evaluation of the fraction in (49) is indistinguishable from 1 for S very close to S_i. If $S_i = 0$, however, the process is stable because the diffusivity term $D(0) = 0$ lets $G(S)$ vanish in the vicinity of S_i. It is obvious that the value of $G(S_i)$ is undefined for all $S_i \in [0, S_0]$, since by definition $F(S_i) = \varphi(S_i) = 0$. We suggest excluding the value of $G(S_i)$ from the discretization of the function G in the numerical computation because $F(S_i) = 0$. Table 5 shows that the number of iterations required to reach machine precision of successive estimates of A increases as $S_0 \to 1$ for both method A and B. This is due to the extremely small difference between the function φ and F in the neighborhood of one, as noted by McWhorter and Sunada (1990). Results given in Table 6 and Figure 3 demonstrate how the function F approaches the Buckley-Leverett-based function F_{BL} introduced in (39). Moreover, convergence also takes place for the first and second derivatives of F, i.e. $F' \to F'_{BL}$ and $F'' \to F''_{BL}$ as $S_0 \to 1$.

The number of iterations increases as $S_0 \to 1$, because the integrals in the iterative scheme determined numerically become inaccurate as limited by the precision of the computer. More importantly, the limit function F_{BL} does not obey the basic assumption that S is a strictly monotone function of λ and its second derivative F''_{BL} is discontinuous. Numerical experiments showed that the function F'', given as

$$F''(S) = -\frac{G(S)}{\int_{S_i}^{S_0} (v - S_i)\, G(v)\, dv} = -G(S)\frac{\Phi(1 - S_{wr} - S_{nr})}{2A^2(1 - Rf(S_i))^2}, \tag{60}$$

is bounded by F''_{BL} (see Figure 3). The convergence of F to F_{BL} as $S_0 \to 1$ can be studied only through numerical experiments since analytical techniques are not available.

For S_0 close to 1, a large number of iterations is needed to achieve convergence of A (see Figure 4). Above a certain value of S_0, the modified iterative process will not converge due to loss of numerical accuracy. However, estimates of the function F and its first and second derivative may converge even though A will not, since the fraction in (44)

$$\frac{\int_{S}^{S_0} (v - S) G_k(v)\, dv}{\int_{S_i}^{S_0} (v - S_i) G_k(v)\, dv}, \tag{61}$$

suppresses any effect of changing A on the function F.

The lower subfigures of Figure 3 indicate that the function G approaches the function F''_{BL}

multiplied by a constant involving A^2 (see (60)). Since $F''_{BL}(S)=0$ for all S in $[S_i,S_t)$, this possible limit function of G as $S_0 \to 1$ does not solve the modified iterative schemes. This is due to $D(S)\neq 0$ in the interval $[S_i,S_t)$, since zero values of G are not admissible in the modified integral equation (47).
Consequently, the integral equation (42) cannot be solved numerically for values of S_0 and R when they are too close to 1.

Method A (48)				
S_0	$\Vert F-F_{BL}\Vert_{L_1}$	$\Vert F'-F'_{BL}\Vert_{L_1}$	$\Vert F''-F''_{BL}\Vert_{L_1}$	Number of iterations
0.6	$5.465648\cdot 10^{-2}$	$2.481441\cdot 10^{-1}$	1.713216	637
0.7	$2.300671\cdot 10^{-2}$	$1.076385\cdot 10^{-1}$	1.211580	1645
0.8	$5.765451\cdot 10^{-3}$	$2.893127\cdot 10^{-2}$	$5.623390\cdot 10^{-1}$	8342
0.9	$1.009092\cdot 10^{-3}$	$5.437080\cdot 10^{-3}$	$1.953441\cdot 10^{-1}$	89684
0.99	$3.759800\cdot 10^{-5}$	$2.194170\cdot 10^{-4}$	$3.099655\cdot 10^{-2}$	10000000*)
0.999	$1.207132\cdot 10^{-5}$	$7.157822\cdot 10^{-5}$	$1.675954\cdot 10^{-2}$	10000000*)
0.9999	$1.068035\cdot 10^{-5}$	$6.345308\cdot 10^{-5}$	$1.554650\cdot 10^{-2}$	10000000*)
Method B (49)				
S_0	$\Vert F-F_{BL}\Vert_{L_1}$	$\Vert F'-F'_{BL}\Vert_{L_1}$	$\Vert F''-F''_{BL}\Vert_{L_1}$	Number of iterations
0.6	$5.465648\cdot 10^{-2}$	$2.481441\cdot 10^{-1}$	1.713216	411
0.7	$2.300671\cdot 10^{-2}$	$1.076385\cdot 10^{-1}$	1.211580	1645
0.8	$5.765451\cdot 10^{-3}$	$2.893127\cdot 10^{-2}$	$5.623390\cdot 10^{-1}$	8348
0.9	$1.009092\cdot 10^{-3}$	$5.437080\cdot 10^{-3}$	$1.953441\cdot 10^{-1}$	89681
0.99	$3.759809\cdot 10^{-5}$	$2.194170\cdot 10^{-4}$	$3.099652\cdot 10^{-2}$	10000000*)
0.999	$1.207278\cdot 10^{-5}$	$7.157773\cdot 10^{-5}$	$1.675853\cdot 10^{-2}$	10000000*)
0.9999	$1.068200\cdot 10^{-5}$	$6.345262\cdot 10^{-5}$	$1.554525\cdot 10^{-2}$	10000000*)

*) the precision $\varepsilon_A = 10^{-15}$ was not reached yet after 10^8 iterations

Table 6. Experimental approaching of $F \to F_{BL}$ as $S_0 \to 1$ for test Setup 1, $S_i = 0$ and $\varepsilon_A = 10^{-15}$.

4.7 Limiting value of A

The convergence of A is an important part of the computational scheme, especially as it depends on S_0. The iterative process may need a large number of iterations for A to converge if S_0 and R are close to one, while the estimates of the function F vary negligibly. Therefore, we pursue the discussion of McWhorter and Sunada (1990), (1992) and Chen et al. (1992) concerning the limit

$$\lim_{S_0 \to 1-} A(S_0). \tag{62}$$

In this section, we consider only the unidirectional displacement case when $R=1$.
McWhorter and Sunada (1990) claimed that the limit (62) is infinite as a consequence of $F \to \varphi$ close to S_0. However, this was questioned by Chen et al. (1992), claiming that the

limit is always finite since the integrand

$$\frac{(v-S_i)D(v)}{F(v)-\varphi(v)} \tag{63}$$

is bounded as $S_0 \to 1$. In the reply to this comment, McWhorter and Sunada (1992) confirmed that the limit (62) is always finite because the integrand (63) is bounded for $v = S_0$. On the other hand, our work shows that the value of A increases without bounds as S_0 approaches 1, as demonstrated in Figure 4. We extend our observations related to F'' approaching F''_{BL} as $S_0 \to 1$ as follows.

The term $\lambda'(S)$ can be evaluated by combining (32) and (36) to yield

$$\frac{\Phi(1-S_{wr}-S_{nr})}{2A(1-f(S_i))}\lambda'(S) = F''(S). \tag{64}$$

We substitute this expression of $\lambda'(S)$ into (29) to obtain

$$\frac{\partial S}{\partial x}(t,x) = \frac{Ag(t)}{2A^2(1-f(S_i))F''(S)}. \tag{65}$$

The total flux condition (25) can be written in the terms of S_0 only, as follows:

$$Ag(t) = Ag(t)f(S_0) - Ag(t)\frac{D(S_0)}{2A^2(1-f(S_i))F''(S_0)}.$$

This equation can be further simplified by employing the S_w formulation into

$$1 = \frac{K\,k_{rw}(S_0)\;p_c(S_0)}{2\mu_w A^2\;(1-f(S_i))F''(S_0)}, \tag{66}$$

and thus one can state

$$\lim_{S_0\to 1} A^2(S_0) = \lim_{S_0\to 1}\frac{K\,k_{rw}(S_0)\;p_c(S_0)}{2\mu_w(1-f(S_i))F''(S_0)}. \tag{67}$$

The limit (67) is infinite for both the Brooks-Corey and van Genuchten models. That is

$$\lim_{S_0\to 1-} A^2(S_0) = +\infty, \tag{68}$$

which agrees with McWhorter and Sunada (1990). Note that the limit (68) is also infinity for the S_n formulation. This result implies that G must be unbounded at some value of S. It can be seen in Figure 3 that G grows dramatically as $S_0 \to 1$ in the region of S_t (the cusp at the front of the Buckley-Leverett shock). Since a cusp has an undefined second derivative, convergence to a cusp implies that the solution is unbounded in the vicinity of the cusp.

5. Solution overview

In this section, we demonstrate how the modified iterative methods using (48) and (49) can delineate the relationship between the McWhorter and Sunada and Buckley-Leverett analytical solutions. We perform computations for Setup 1 with $S_i = 0$ with various values of R and S_0. In order to compare the McWhorter and Sunada exact solution (37) with the Buckley-Leverett analytical solution (13), we use the value of A corresponding to the McWhorter and Sunada exact solution for $R = 1$.

Figure 5 shows how the cases of bi-directional displacement (R=0, diffusive term only in (11)), partially unidirectional displacement (R=0.8, both advective and diffusive terms in (11)), and unidirectional displacement (R=1, both advective and diffusive terms in (11)) are related to the Buckley-Leverett solution of the advection equation (12). As S_0 approaches 1, the diffusive term in (11) has less effect on the solution. Table 7 displays values of A for various combinations of R and S_0.

The modified iterative process allows solutions for strongly advective terms in (11), whereas the original iterative process fails in situations where the diffusive term is still significant. Since the critical value S_0^* for Setup 1 with $S_i = 0$ and $R = 1$ is $S_0^* = 0.69$, solutions with $R = 1$ shown in Figure 5, except the case $S_0 = 0.6$, are only obtainable by our modified iterative method.

Dependency of A on S_0 and R						
S_0	R=0	R=0.2	R=0.4	R=0.6	R=0.8	R=1
0.40	$1.372282 \cdot 10^{-4}$	$1.422307 \cdot 10^{-4}$	$1.481100 \cdot 10^{-4}$	$1.552003 \cdot 10^{-4}$	$1.640657 \cdot 10^{-4}$	$1.757718 \cdot 10^{-4}$
0.50	$1.758601 \cdot 10^{-4}$	$1.858937 \cdot 10^{-4}$	$1.987728 \cdot 10^{-4}$	$2.164222 \cdot 10^{-4}$	$2.435723 \cdot 10^{-4}$	$2.984027 \cdot 10^{-4}$
0.60	$1.977760 \cdot 10^{-4}$	$2.114149 \cdot 10^{-4}$	$2.297735 \cdot 10^{-4}$	$2.569444 \cdot 10^{-4}$	$3.056894 \cdot 10^{-4}$	$4.879118 \cdot 10^{-4}$
0.70	$2.082277 \cdot 10^{-4}$	$2.237585 \cdot 10^{-4}$	$2.451182 \cdot 10^{-4}$	$2.779105 \cdot 10^{-4}$	$3.417753 \cdot 10^{-4}$	$8.879432 \cdot 10^{-4}$
0.80	$2.121827 \cdot 10^{-4}$	$2.284708 \cdot 10^{-4}$	$2.510610 \cdot 10^{-4}$	$2.862575 \cdot 10^{-4}$	$3.572659 \cdot 10^{-4}$	$2.027109 \cdot 10^{-3}$
0.90	$2.131235 \cdot 10^{-4}$	$2.295997 \cdot 10^{-4}$	$2.525009 \cdot 10^{-4}$	$2.883224 \cdot 10^{-4}$	$3.613094 \cdot 10^{-4}$	$5.474154 \cdot 10^{-3}$
0.99	$2.131881 \cdot 10^{-4}$	$2.296778 \cdot 10^{-4}$	$2.526013 \cdot 10^{-4}$	$2.884687 \cdot 10^{-4}$	$3.616068 \cdot 10^{-4}$	$3.276546 \cdot 10^{-2}$

Table 7. Values of A for various values of R and S_0; test Setup 1, $S_i = 0$, M=10000 nodes.

6. Conclusions

The article is devoted to a detailed discussion of the benchmark solution described by McWhorter and Sunada (1990). We propose a reliable procedure for solving the implicit functional relationship that is the result of the analytical treatment of the advection-diffusion equation. This algorithm extends the use of the semi-analytical approach to a wider range of entry saturations than the original algorithm proposed by McWhorter and Sunada (1990). The use of our algorithm is limited by the round-off errors of the numerical computations and the number of iterations required for solution.

From our analysis, it follows that the original iterative method proposed by McWhorter and Sunada (1990) can be used to obtain solutions of the unidirectional displacement problem (R=1) only in a restricted interval of the entry saturations S_0. The restricted interval can be determined by examining the first iteration. Our modified iterative method removes this restriction and offers a solution for larger range of entry saturations.

Method A (equation (48)) can be used to compute the solution for any admissible parameters except the values of S_0 and R extremely close to 1 while method B (equation (49)) randomly fails if $S_i > 0$. Therefore, the iterative method described by method A (equation (48)) can be used exclusively for use of the McWhorter and Sunada quasi-analytical solution.

The comparison of the McWhorter-Sunada fractional flow function F with the Buckley-Leverett fractional flow function, F_{BL}, allows us to determine the limit of A as $S_0 \to 1$ and therefore to confirm the statement given by McWhorter and Sunada (1990), in contrast to the contentions of Chen et al. (1992) and McWhorter and Sunada (1992).

The practical value of our results is that they contribute to a detailed analysis of the analytical benchmark solution often useful for verification of more complex numerical models and in providing a tool for comparison under conditions of high wetting-phase saturations. Such a code verification was conducted by Mikyška and Illangasekare (2005) where this improved solution was used.

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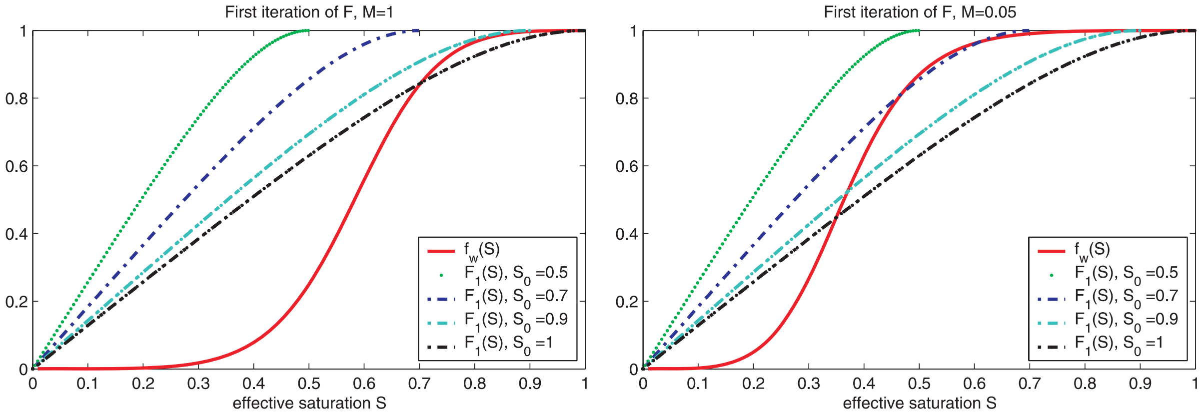


Figure 1. Graphs of the function φ and F_1 for different choices of S_0 illustrate why the original iterative process fails after the first iteration. Brooks-Corey model uses $\lambda = 2$.

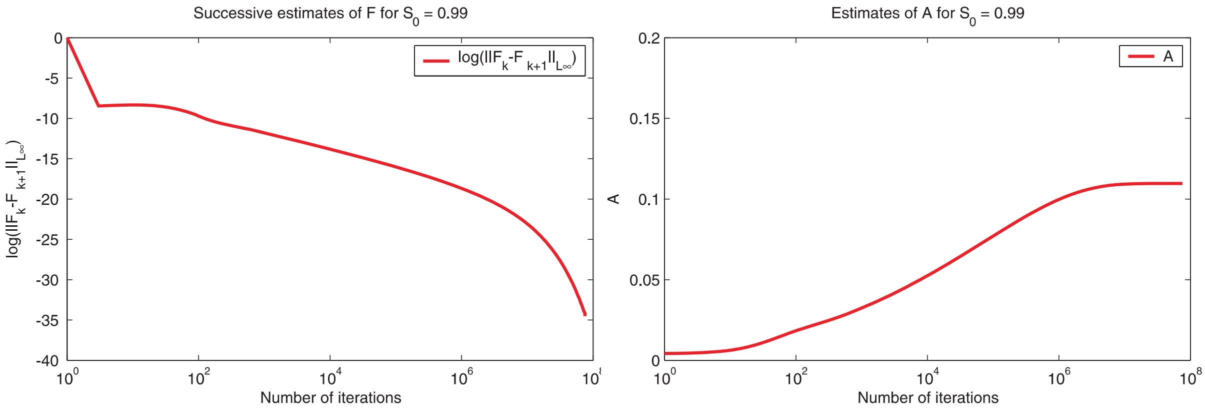


Figure 2. Illustration of successive approximations of F in the L_∞ norm (using the decadic logarithmic scale) and the value of A. We used the method A (48), Setup 1 with $S_i = 0$ and $S_0 = 0.99$. The iterative process is terminated by $\varepsilon_A = 10^{-15}$.

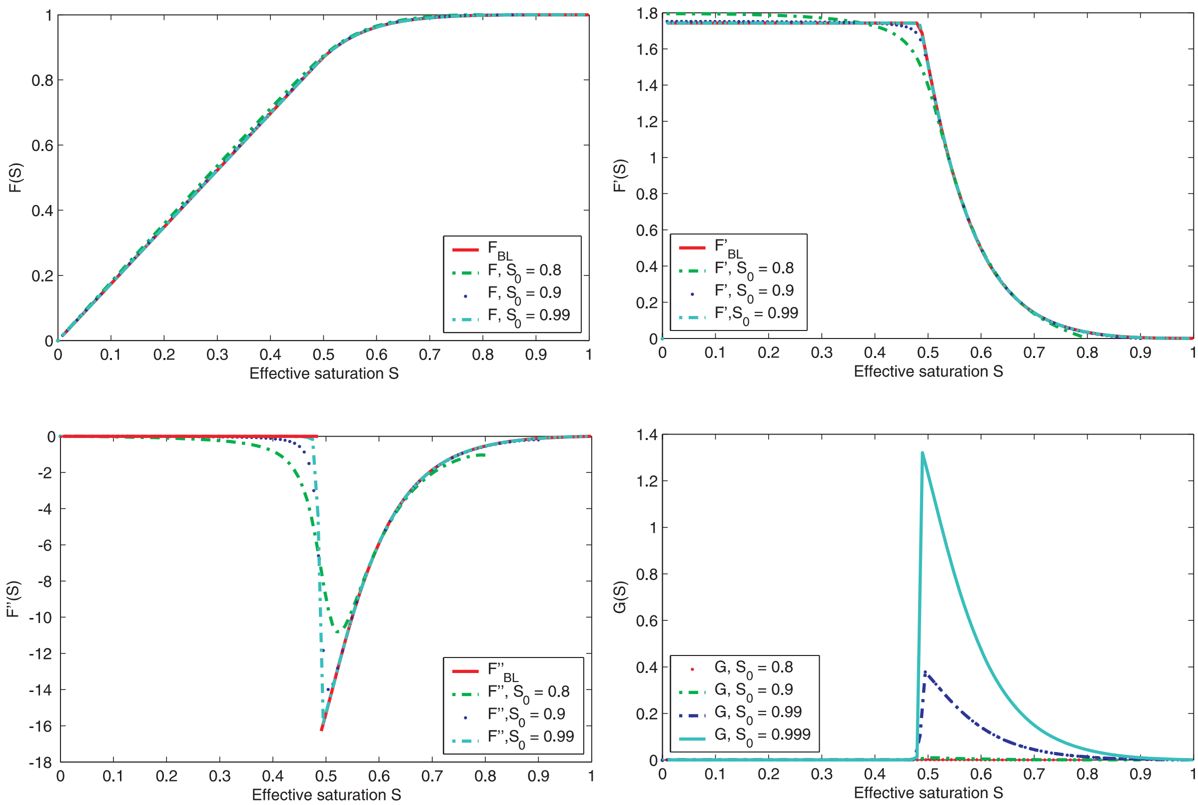


Figure 3. Experimental convergence of the functions F to F_{BL}, F' to F'_{BL} and F'' to F''_{BL} as $S_0 \to 1$ for Setup 1 with $S_i = 0$, using method A (48). The last figure depicts the evolution of the function G as $S_0 \to 1$. Note that the function G and F'' are related by (60), i.e. they differ only by a factor involving A^2.

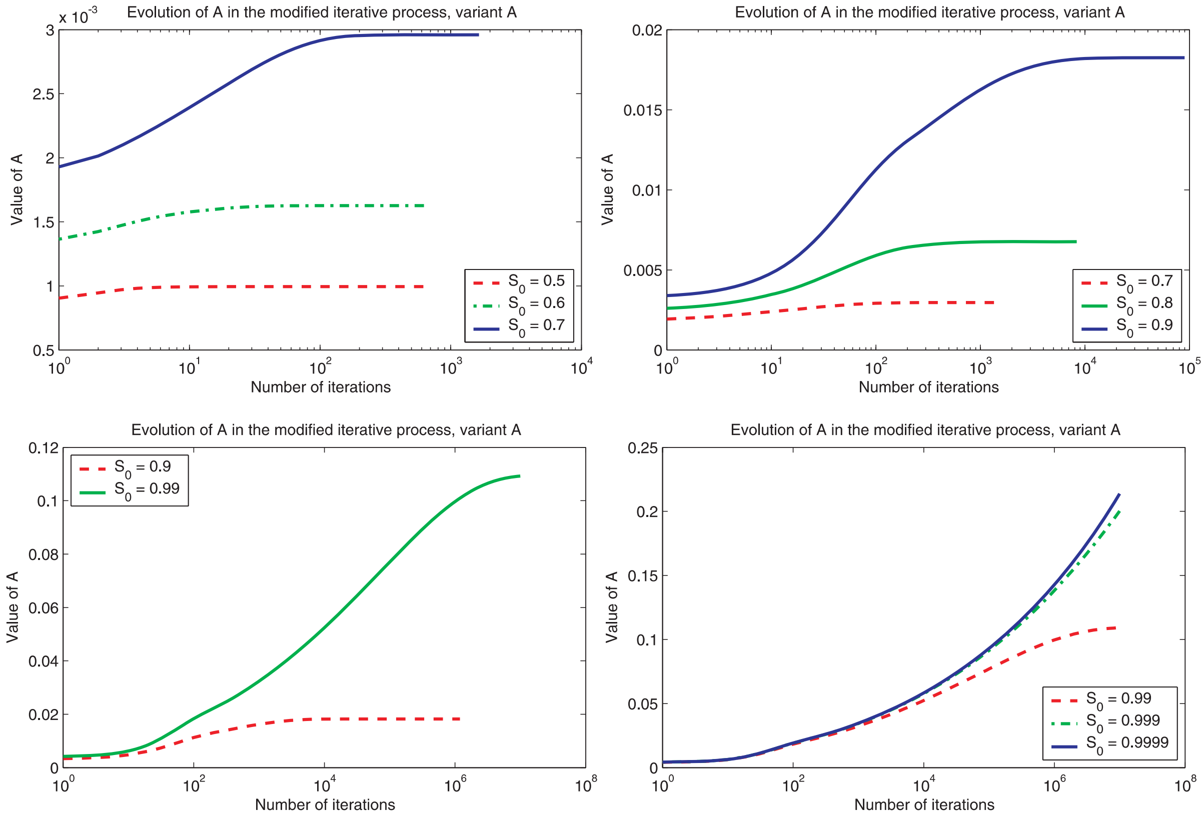


Figure 4. Evolution of A in the modified iterative process, method A; test Setup 1, $S_i = 0$. As S_0 approaches 1, the iterative process requires higher number of iterations to reach convergence of A. In the very proximity of $S_0 = 1$, the value of A is far from convergence even after 10^8 iterations. The situation for the method B is analogous.

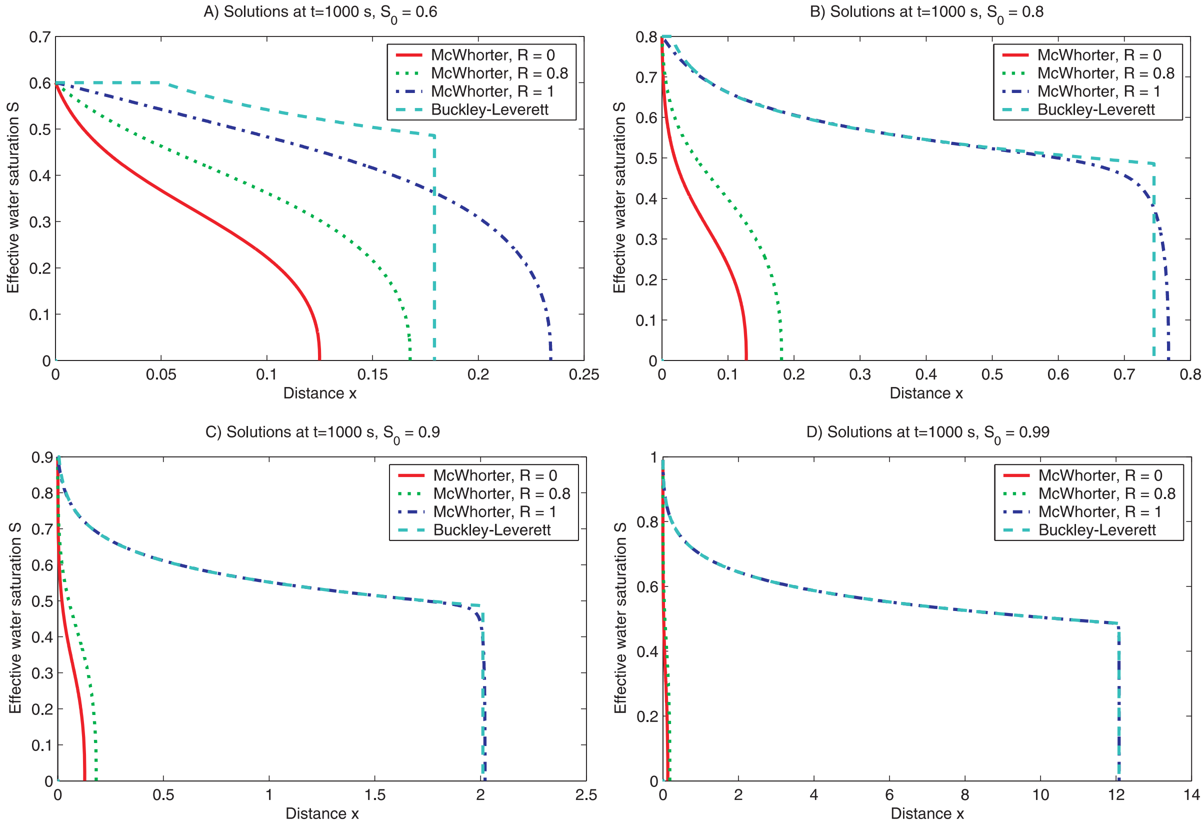


Figure 5. McWhorter exact solutions (the method A) and Buckley-Leverett analytical solutions for various S_0; test Setup 1, $S_i = 0$. As $S_0 \to 1$, the unidirectional displacement solution (R=1) approaches the Buckley-Leverett solution, while the head of the bi-directional displacement solution (R=0) advances negligibly.

Figures

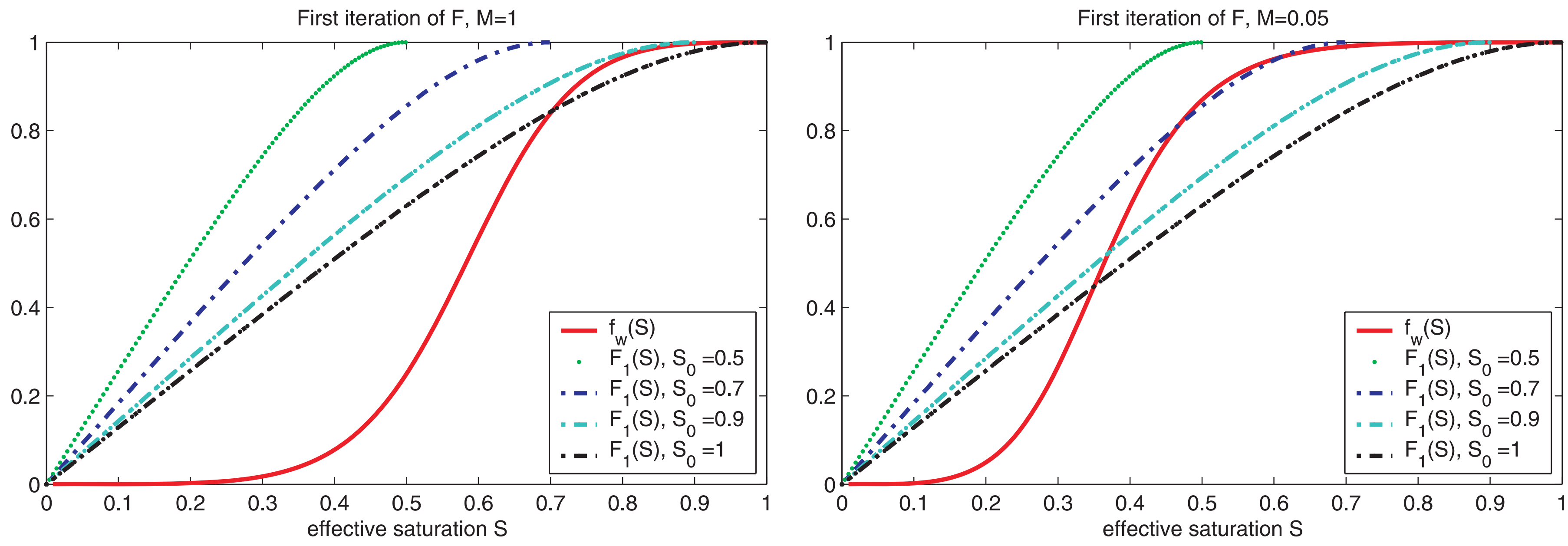

First iteration of F, M=1
First iteration of F, M=0.05
effective saturation S
effective saturation S
f_w(S)
F_1(S), S_0 =0.5
F_1(S), S_0 =0.7
F_1(S), S_0 =0.9
F_1(S), S_0 =1

Figure 1

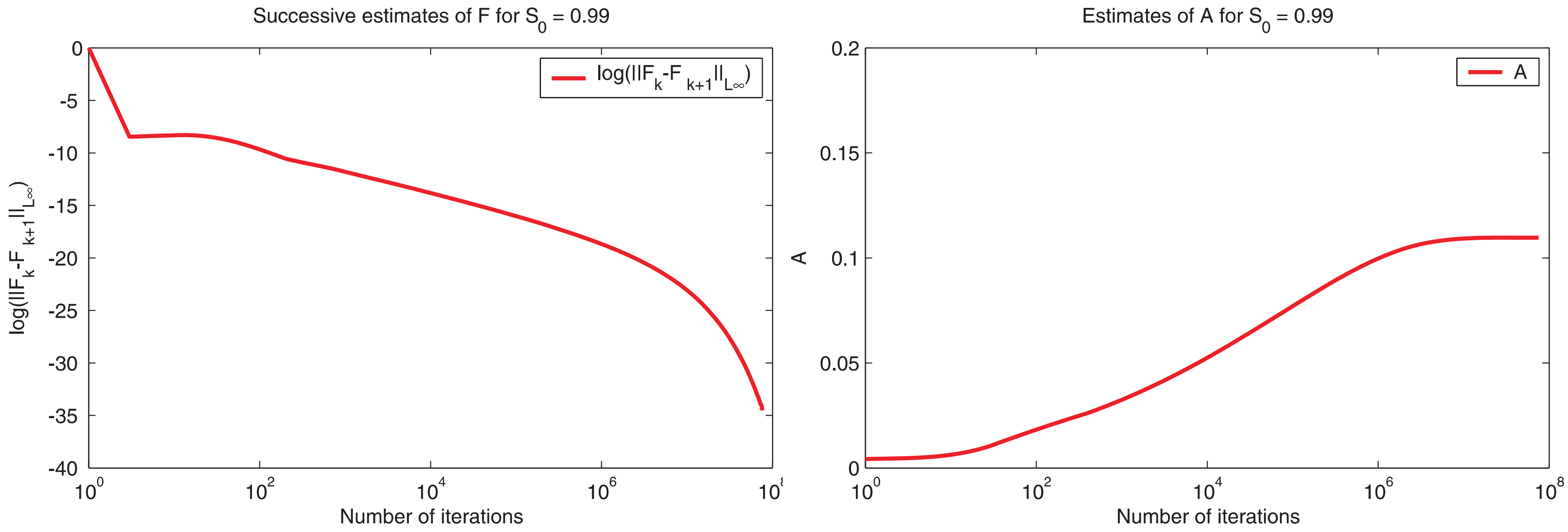

Successive estimates of F for S0 = 0.99
log(||Fk-F k+1||L∞)
Number of iterations
Estimates of A for S0 = 0.99
A
Number of iterations

Figure 2

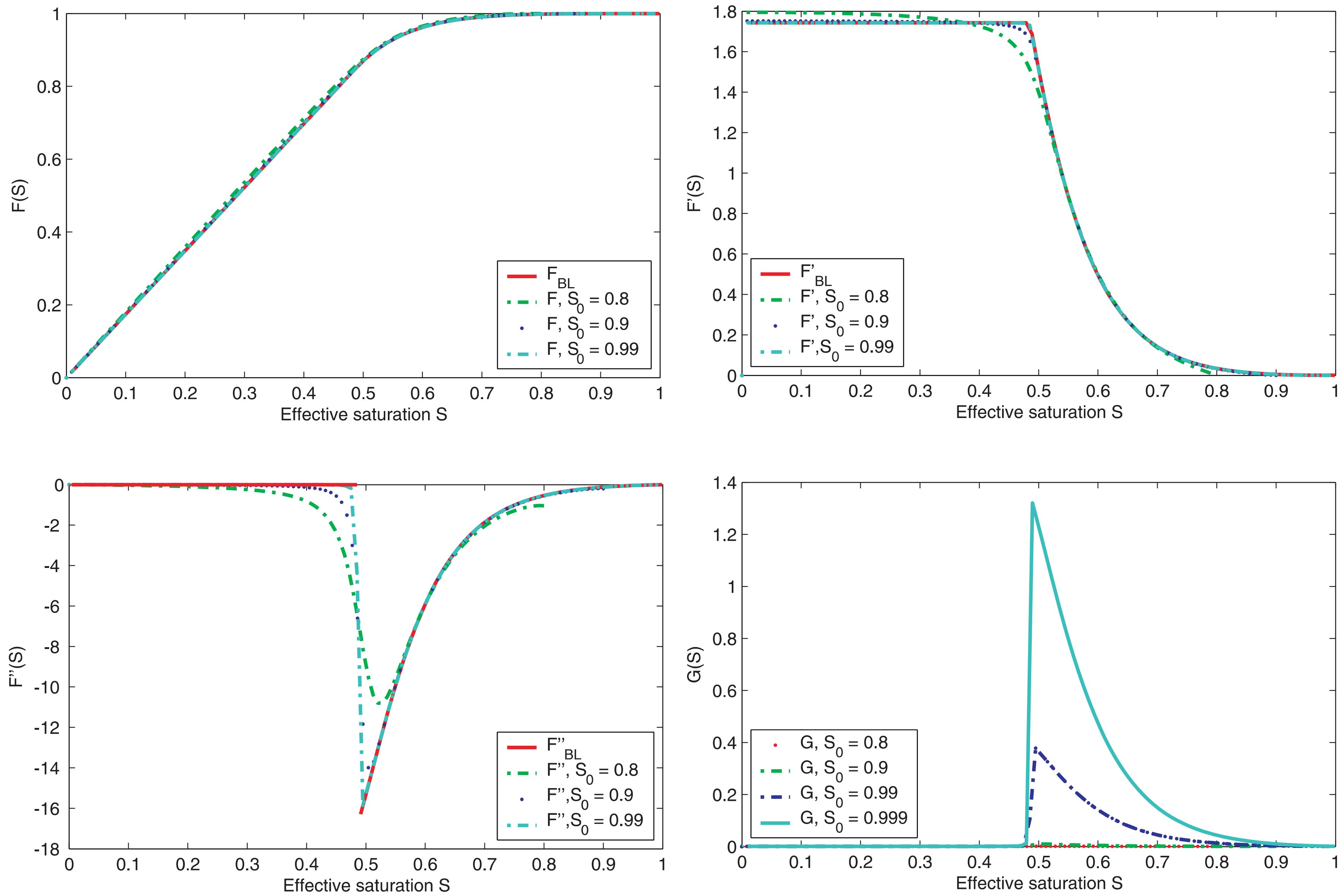

F(S)
Effective saturation S
F_BL
F, S_0 = 0.8
F, S_0 = 0.9
F, S_0 = 0.99
F'(S)
F'_BL
F', S_0 = 0.8
F', S_0 = 0.9
F',S_0 = 0.99
F''(S)
F''_BL
F'', S_0 = 0.8
F'',S_0 = 0.9
F'',S_0 = 0.99
G(S)
G, S_0 = 0.8
G, S_0 = 0.9
G, S_0 = 0.99
G, S_0 = 0.999

Figure 3

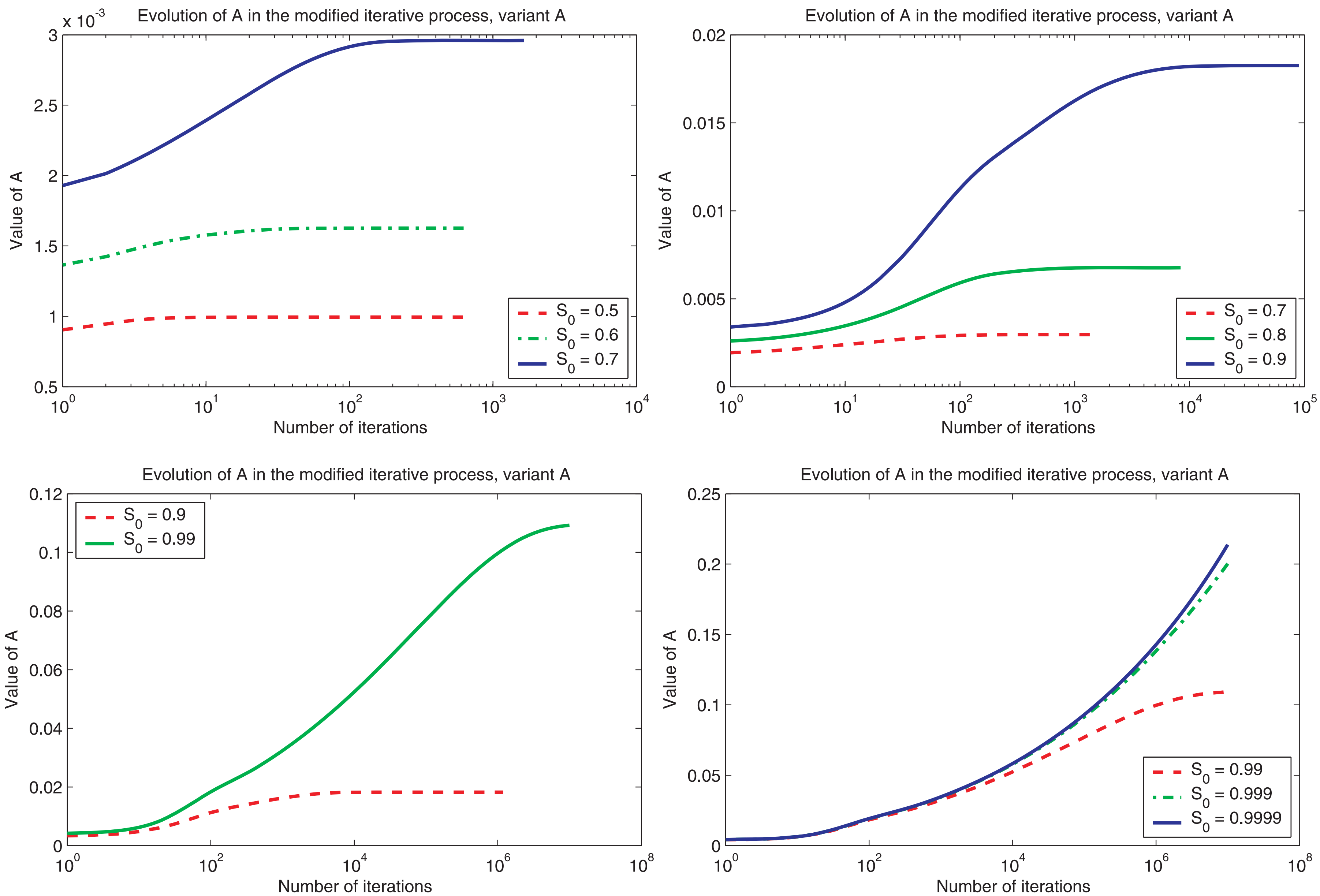
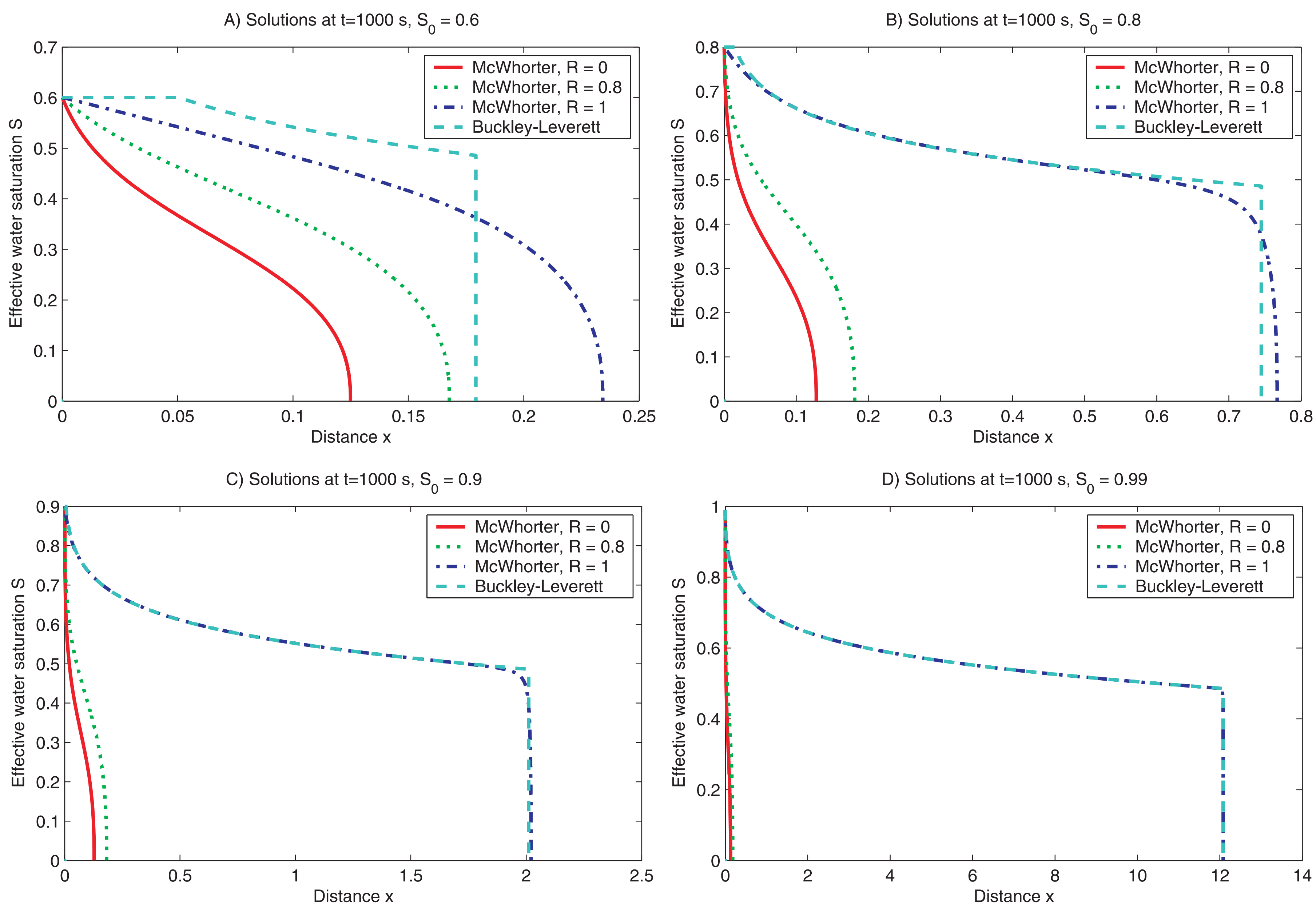

Evolution of A in the modified iterative process, variant A
x 10^-3
Value of A
Number of iterations
S0 = 0.5
S0 = 0.6
S0 = 0.7
Evolution of A in the modified iterative process, variant A
Value of A
Number of iterations
S0 = 0.7
S0 = 0.8
S0 = 0.9
Evolution of A in the modified iterative process, variant A
Value of A
Number of iterations
S0 = 0.9
S0 = 0.99
Evolution of A in the modified iterative process, variant A
Value of A
Number of iterations
S0 = 0.99
S0 = 0.999
S0 = 0.9999

Figure 4



A) Solutions at t=1000 s, S0 = 0.6
B) Solutions at t=1000 s, S0 = 0.8
C) Solutions at t=1000 s, S0 = 0.9
D) Solutions at t=1000 s, S0 = 0.99
Effective water saturation S
Distance x
McWhorter, R = 0
McWhorter, R = 0.8
McWhorter, R = 1
Buckley-Leverett

Figure 5