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A pseudospectral approach to the McWhorter and Sunada equation for two-phase flow in porous media with capillary pressure

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Abstract Two well known mathematical solutions for two-phase flow in porous media are the Buckley-Leverett equation and the McWhorter and Sunada equation (MSE). The former ignores capillary pressure and can be solved analytically. The latter has traditionally been formulated as an iterative integral solution, which suffers from convergence problems as the injection saturation approaches unity. Here an alternative approach is presented that solves the MSE using a pseudospectral Chebyshev differentiation matrix. The resulting pseudospectral solution is compared to results obtained from the original integral implementation and the Buckley-Leverett limit, when the capillary pressure becomes negligible. A self-contained MATLAB code to implement the new solution is provided within the manuscript. The new approach offers a robust and accurate method for verification of numerical codes solving two-phase flow with capillary pressure.

1 Introduction

Analytical solutions are often used to help verify numerical simulation of flow and transport in porous media. Buckley and Leverett [3] derived such an analytical solution to look at the saturation distribution resulting from one-dimensional immiscible two-phase flow in porous media in the absence of capillary pressure. This solution has been extended by many researchers to account for partially miscible displacement [see 9, and references therein]. More recently, Mathias et al [7] provided an analytical solution to describe the pressure distribution resulting from a partially miscible two-phase displacement in a radial flow-field but also ignoring capillary pressure.

Such solutions have been possible because the ignoring of capillary pressure leads to a hyperbolic partial differentiation equation, which can be solved using similarity transforms and the method of characteristics [9]. However, when capillary pressure is accounted for, the equations become diffusive, resulting in the problem not being generally self-similar, except when the boundary flux is inversely proportional to the square root of time [8]. Having applied such a boundary condition, McWhorter and Sunada [8] reduced the governing equations for one-dimensional immiscible two-phase flow in porous media in the presence of capillary pressure to a single non-linear second-order ordinary differential equation, hereafter referred to as the McWhorter and Sunada equation (MSE). The MSE can be considered as the capillary effect analogue of the Buckley-Leverett solution for viscous dominated flow [13]. Note that there are several additional solutions for two-phase flow in porous media with capillary pressure that do not involve the MSE (see Table 2 of Schmid and Geiger, [13]). However, these generally involve restricting the functional form of the capillary pressure function and/or the relative permeability functions.

Applications of the MSE go beyond the verification of other numerical codes. By comparing

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with the Buckley-Leverett equation, the MSE can be used to evaluate the impact of capillary pressure, similar to work done by Goumiri et al [5]. The MSE also forms the starting point of a new set of semi-analytical solutions to consider hydrodynamic dispersion and adsoprtion of solutes in two-phase flow [see 14, 15]. More recently, the MSE has been used to derive a new scaling group for interpretation and upscaling of laboratory experiments associated with spontaneous, counter-current imbibition [13].

McWhorter and Sunada [8] present an exact solution to their boundary value problem in the form of an iterative integral equation. Despite much effort to improve the iterative procedure [4], convergence of the solution has proven to be very sensitive to the relative permeabilities and viscosities of the fluids for large wetting saturations at the inlet. The purpose of this article is to propose a more robust approach for solving the MSE, involving the use of pseudospectral differentiation matrices [17, 11]. Pseudospectral methods are known to have the capability to provide an exponential rate of convergence as the grid is refined [6], particularly when the solution is smooth [11]. With the exception of van Reeuwijk et al [12], pseudospectral methods have attracted little attention in the porous media literature. Nevertheless, such an approach is likely to be useful for a range of different porous media applications.

The outline of the article is as follows. A normalized form of the self-similar MSE is derived. Then, closely following the work of Piche and Kanniainen [11], a solution procedure using a Chebyshev differentiation matrix is presented. A self-contained MATLAB code is provided to evaluate the worked examples previously studied by McWhorter and Sunada [8]. Finally, following Fucik et al [4], the pseudospectral solution is further verified by comparison with the Buckley-Leverett equation, as the capillary pressure becomes negligibly small.

2 Governing equations

Consider the governing equations for one-dimensional, horizontal (ignoring gravity), two-phase incompressible and immiscible displacement in a rigid and homogeneous porous medium. The mass balance equations for the two phases considered reduce to:

$$\phi\frac{\partial S_w}{\partial t} = -\frac{\partial q_w}{\partial x} \tag{1}$$

$$\phi\frac{\partial S_n}{\partial t} = -\frac{\partial q_n}{\partial x} \tag{2}$$

where ϕ [$-$] is the porosity, t [T] is time, x [L] is distance, S_w [-] and S_n [-] are the volumetric fluid saturations of the wetting and non-wetting phase, respectively, and q_w [LT^{-1}] and q_n [LT^{-1}] are the volumetric flow rates per unit area for the wetting and non-wetting phase, respectively, defined by Darcy's law:

$$q_w = -k\frac{k_{rw}}{\mu_w}\frac{\partial p_w}{\partial x} \tag{3}$$

$$q_n = -k\frac{k_{rn}}{\mu_n}\frac{\partial p_n}{\partial x} \tag{4}$$

where k [L^2] is the intrinsic permeability and k_{rw} [-], μ_w [ML^{-1}T^{-1}], p_w [ML^{-1}T^{-2}], k_{rn} [-], μ_n [ML^{-1}T^{-1}], and p_n [ML^{-1}T^{-2}] are the relative permeability, dynamic viscosity and fluid pressure for the wetting and non-wetting phases, respectively. In addition, the saturations, flow rates and fluid pressures for both phases are related by the following expressions:

$$S_n + S_w = 1 \tag{5}$$

$$q_t = q_n + q_w \tag{6}$$

$$p_w = p_n - p_c \tag{7}$$

where q_t [LT^{-1}] is the total volumetric flow rate per unit area and p_c [ML^{-1}T^{-2}] is the capillary pressure. Note that due to the assumption of incompressible fluids and rigid porous medium, q_t does not vary with position x, but is constant everywhere.

2.1 Reduction to a single partial differential equation

Substituting Eq. (7) into Eq. (3) and assuming that $p_c = p_c(S_w)$ yields

$$q_w = -k\frac{k_{rw}}{\mu_w}\frac{\partial p_n}{\partial x} - q_c \tag{8}$$

where

$$q_c = -k\frac{k_{rw}}{\mu_w}\frac{dp_c}{dS_w}\frac{\partial S_w}{\partial x} \tag{9}$$

Then, substituting Eqs. (8) and (4) into Eq. (6) leads to

$$q_t = -k\left(\frac{k_{rw}}{\mu_w}+\frac{k_{rn}}{\mu_n}\right)\frac{\partial p_n}{\partial x} - q_c \tag{10}$$

It can now be seen that

$$\frac{q_w+q_c}{q_t+q_c} = f_w \tag{11}$$

where (consider Buckley and Leverett [3])

$$f_w = \left(1+\frac{k_{rn}\mu_w}{k_{rw}\mu_n}\right)^{-1} \tag{12}$$

Defining the ratio γ:

$$\gamma \equiv \frac{q_t}{q_{w0}} \tag{13}$$

where $q_{w0} = q_w(0,t)$ is the volumetric flow rate of the wetting phase per unit area at the injection point. Rearranging Eq. (11) and using (13), leads to

$$q_w = q_{w0}\gamma f_w - (1-f_w)q_c \tag{14}$$

and from Eq. (1), it can then be said that

$$\phi\frac{\partial S_w}{\partial t} = -q_{w0}\frac{\partial F_w}{\partial x} \tag{15}$$

where the fractional flow ratio F_w is defined as:

$$F_w \equiv \frac{q_w}{q_{w0}} = \gamma f_w + \frac{G}{q_{w0}}\frac{\partial S_w}{\partial x} \tag{16}$$

and

$$G = \frac{k f_w k_{rn}}{\mu_n}\frac{dp_c}{dS_w} \tag{17}$$

Note that $(1-f_w)k_{rw}/\mu_w = f_w k_{rn}/\mu_n$. Note also that for unidirectional flow ($q_t = q_{w0}$, i.e., $\gamma = 1$), by ignoring capillary pressure (i.e., by setting $G = 0$), Eq. (15) reduces to the Buckley-Leverett displacement equation [3].

McWhorter and Sunada [8] consider the following initial and boundary conditions for unidirectional flow case:

$$\begin{aligned} &S_w = S_{wi},\ x>0,\ \ t=0\\ &q_w = q_{w0},\ x=0,\ \ t\geq 0\\ &S_w = S_{wi},\ x\to\infty,\ t\geq 0 \end{aligned} \tag{18}$$

2.2 Reduction to an ordinary differential equation

As discussed in the introduction, the above set of equations become self-similar when

$$q_{w0} = At^{-1/2} \tag{19}$$

where A is a constant [LT$^{-1/2}$], which is often linked to the ability of a porous medium to imbibe fluid at the boundary [13].

Substitution of Eq. (19) into Eq. (15) and applying the similarity transform

$$\lambda = xt^{-1/2} \tag{20}$$

leads to the ordinary differential equation:

$$\frac{2A}{\phi}\frac{dF_w}{dS_w} = \lambda \tag{21}$$

From Eq. (16) we get that

$$\frac{G}{A}\frac{1}{(F_w-\gamma f_w)} = \frac{d\lambda}{dS_w} \tag{22}$$

and differentiating both sides of Eq. (21) with respect to S_w yields

$$\frac{2A}{\phi}\frac{d^2F_w}{dS_w^2} = \frac{d\lambda}{dS_w} \tag{23}$$

from which it follows that

$$\frac{d^2F_w}{dS_w^2} = \frac{\phi G}{2A^2}\frac{1}{(F_w-\gamma f_w)} \tag{24}$$

The initial and boundary conditions in Eq. (18) reduce to

$$\begin{aligned} &F_w = F_{w0},\ S_w = S_{w0}\\ &F_w = F_{wi},\ \ S_w = S_{wi} \end{aligned} \tag{25}$$

where

$$F_{w0} = 1, \quad F_{wi} = \gamma f_{wi} \tag{26}$$

and $f_{wi} = f_w(S_{wi})$ and S_{w0} and F_{w0} are defined as the value of S_w and F_w at $x = 0$, respectively, for a given value of A. Note that F_{w0} is always equal to 1. In practice, a value of S_{w0} is specified and the corresponding value of A is found iteratively [8].

2.3 Application of dimensionless transforms

Here we introduce a dimensionless transformation of A, defined as:

$$A_D = A\left(\frac{2\mu_w}{\phi k p_e}\right)^{1/2} \tag{27}$$

where p_e [$\mathrm{ML^{-1}T^{-2}}$] is a characteristic capillary pressure. Eqs. (21) and (24) then reduce to

$$\frac{dF_w}{dS_w} = \lambda_D \tag{28}$$

$$\frac{d^2F_w}{dS_w^2} = \frac{G_D}{A_D^2}\frac{1}{(F_w-\gamma f_w)} \tag{29}$$

where

$$G_D = f_w k_{rn} Mo\frac{dp_{cD}}{dS_w}, \quad \lambda_D = \frac{\lambda}{A_D}\left[\frac{\phi}{2}\frac{\mu_w}{kp_e}\right]^{1/2} \tag{30}$$

and

$$p_{cD} = \frac{p_c}{p_e}, \quad Mo = \frac{\mu_w}{\mu_n} \tag{31}$$

3 McWhorter and Sunada integral solution

Eq. (29) can be integrated twice to obtain:

$$\begin{aligned} F_w = K_1\frac{S_w-S_{wi}}{S_{w0}-S_{wi}} \\ -\frac{1}{A_D^2}\left[\left(1-\frac{S_w-S_{wi}}{S_{w0}-S_{wi}}\right)\int_{S_{wi}}^{S_{w0}}\frac{(S_w-S_{wi})G_D}{F_w-\gamma f_w}dS_w\right. \\ \left. -\int_{S_w}^{S_{w0}}\frac{(\beta-S_w)G_D}{F_w-\gamma f_w}d\beta\right] + K_2 \end{aligned} \tag{32}$$

where

$$K_1 = F_{w0}, \quad K_2 = \left(1-\frac{S_w-S_{wi}}{S_{w0}-S_{wi}}\right)F_{wi} \tag{33}$$

where F_{wi} is F_w at $x=0$. Differentiating Eq. (32) leads to:

$$\begin{aligned} \frac{dF_w}{dS_w} = \frac{1}{S_{w0}-S_{wi}} \\ \cdot\left(F_{w0}+\frac{1}{A_D^2}\int_{S_{wi}}^{S_{w0}}\frac{(S_w-S_{wi})G_D}{F_w-\gamma f_w}dS_w - F_{wi}\right) \\ -\frac{1}{A_D^2}\int_{S_w}^{S_{w0}}\frac{G_D}{F_w-\gamma f_w}d\beta \end{aligned} \tag{34}$$

and imposing that $dF_w/dS_w = 0$ at $S_w = S_{w0}$ and using Eq. (25) gives:

$$A_D^2 = \frac{1}{F_{wi}-F_{w0}}\int_{S_{wi}}^{S_{w0}}\frac{(S_w-S_{wi})G_D}{F_w-\gamma f_w}dS_w \tag{35}$$

The solution algorithm described by McWhorter and Sunada [8] is to solve the integral Eq. (32) for F $(=(F_w-\gamma f_{wi})/(1-\gamma f_{wi}))$ and a non-normalized form of Eq. (35) sequentially in an iterative loop until F converges to a solution which occurs when successive iterations are sufficiently small in a norm. Unfortunately, convergence of the solution process is very sensitive to the injection saturation, S_{w0} when it approaches unity, causing the iteration routine to fail. Fucik et al [4] improved on this process, but it still requires a large number of iterations to converge.

4 Chebyshev spectral collocation (pseudospectral) method

The main motivation and purpose of this article, is to introduce an alternative approach to find a more robust and accurate solution of F_w using a pseudospectral differentiation matrix. Instead of evaluating the integral equation in Eq. (32), the boundary value problem defined by Eqs. (29) and (25) is solved using a differentiation matrix, $\mathbf{D}$, which is a matrix such that the values of the d'th derivative of a function $y(\mathbf{x})$ at distinct nodes $\mathbf{x}$ can be approximated by $y^{(d)}(\mathbf{x}) \approx \mathbf{D}^{(d)}y(\mathbf{x})$. Using appropriate formulae, $\mathbf{D}$ can be obtained for various discretization schemes (finite difference, Chebyshev, Fourier etc.), making it straightforward to switch between various polynomial methods [17, 11]. But, as in van Reeuwijk et al [12], the nonperiodicity of the boundary conditions suggest the use of an expansion in Chebyshev polynomials [2, p. 10].

The Chebyshev spectral collocation (pseudospectral) method results in a denser differentiation matrix compared to the normally sparse matrices of the finite difference method. However, when the data defining the problem are smooth, they can often achieve as much as ten digits of accuracy where a finite difference method would get just two or three [16, 11]. At lower accuracies, they demand less computer memory than the alternatives and should, for that reason, often be a preferable method.

The Chebyshev polynomial of the second kind, p, interpolates a function, y, at the nodes (so-called Chebyshev points) [17, p. 479]

$$\mathbf{x}_k = \cos\left(\frac{(k-1)\pi}{N-1}\right), \quad k = 1,2,\ldots,N \tag{36}$$

such that $p(\mathbf{x}) = y(\mathbf{x})$. Note that $x \in [-1,1]$.

The value of the interpolating polynomial's d'th derivative at the k'th node is given by [17]:

$$p^{(d)}(\mathbf{x}) = \mathbf{D}^{(d)} y(\mathbf{x}) \tag{37}$$

where $\mathbf{D}^{(d)}$ is the d'th order Chebyshev differentiation matrix. A short MATLAB code for creating Chebyshev points, $\mathbf{x}$, and differentiation matrix, $\mathbf{D}$, is given by Trefethen [16, p. 54], an alternative code using various strategies for enhanced accuracy is provided by Weideman and Reddy [17].

In the differentiation matrix method for solving differential equations, the interpolating polynomial is only required to satisfy the differential equation at the interior nodes. The values at the interpolating polynomial and the derivatives at the interior nodes are, respectively (consider [11]):

$$p(\mathbf{x}_{2:N-1}) = y(\mathbf{x}_{2:N-1}) = \mathbf{I}_{2:N-1,:}\mathbf{y} \tag{38}$$

$$p^{(d)}(\mathbf{x}_{2:N-1}) = \mathbf{D}^{(d)}_{2:N-1,:}\mathbf{y} \tag{39}$$

where $\mathbf{I}$ is the identity matrix.

Boundary conditions are given as constraints for Dirichlet boundary conditions and derivatives for Neumann boundary conditions and are defined on the end nodes, corresponding to the first and last rows of the differentiation matrix:

$$\begin{aligned} \text{Dirichlet:} \quad & p(x=1) = \mathbf{y}_1 \\ & p(x=-1) = \mathbf{y}_N \end{aligned} \tag{40}$$

$$\begin{aligned} \text{Neumann:} \quad & p^{(d)}(x=1) = \mathbf{D}^{(d)}_{1,:}\mathbf{y} \\ & p^{(d)}(x=-1) = \mathbf{D}^{(d)}_{N,:}\mathbf{y} \end{aligned} \tag{41}$$

5 Pseudospectral solution of the McWhorter-Sunada equation

Recall that the coordinate space for the Chebyshev nodes is $x \in [-1,1]$ (note that $\mathbf{x}_N = -1$ and $\mathbf{x}_1 = 1$). But the solution space for the saturation is $S_w \in [S_{wi}, S_{w0}]$. Therefore the Chebyshev nodes, $\mathbf{x}_k$, need to be mapped to the saturation space by the following transform:

$$S_w = \frac{S_{w0} + S_{wi}}{2} + \frac{S_{w0} - S_{wi}}{2} x \tag{42}$$

Hence, we introduce an appropriately transformed differentiation matrix, $\mathbf{E}$, where

$$\mathbf{E} = \frac{dx}{dS_w}\mathbf{D} \tag{43}$$

and from Eq. (42)

$$\frac{dx}{dS_w} = \frac{2}{S_{w0} - S_{wi}} \tag{44}$$

By applying Eq. (39) on the interior nodes and Dirichlet boundary conditions, Eq. (40), on the end-nodes, Eq. (29) can be written in matrix form (similar to [11]):

$$\mathbf{R}(\mathbf{F}) = \begin{bmatrix} \mathbf{E}^{(2)}_{2:N-1,:}\mathbf{F} - \mathbf{I}_{2:N-1,:}\left[\dfrac{G_D}{A_D^2(F_w - \gamma f_w)}\right] \\ \mathbf{F}_N - F_{wi} \\ \mathbf{F}_1 - F_{w0} \end{bmatrix} \tag{45}$$

where $\mathbf{R}$ is the residual vector, $\mathbf{F}$ represents the solution vector for the dependent variable F_w and the two last rows impose the Dirichlet boundary conditions, Eq. (25), on F_w.

5.1 Newton's method

Using Newton's method, the solution vector $\mathbf{F}$ can be found by minimizing the ℓ^2-norm of the residual vector in Eq. (45), and in each iteration, i, the value of the solution vector is updated by the following statement:

$$\mathbf{F}_{(i+1)} = \mathbf{F}_i - (\partial\mathbf{R}/\partial\mathbf{F}_i)^{-1}\,\mathbf{R}(\mathbf{F}_i) \tag{46}$$

where $\partial\mathbf{R}/\partial\mathbf{F}$ is the Jacobian matrix defined as:

$$\frac{\partial\mathbf{R}}{\partial\mathbf{F}} = \begin{bmatrix} \mathbf{E}^{(2)}_{2:N-1,;} - \mathbf{I}_{2:N-1,;}\text{diag}\left[-\dfrac{G_D}{A_D^2(F_w - \gamma f_w)^2}\right] \\ \mathbf{I}_{N,:} \\ \mathbf{I}_{1,:} \end{bmatrix} \tag{47}$$

Note that F_w is bounded by f_w and F_{w0} such that $\gamma f_w < F_w \leq F_{w0}$. Therefore a good initial guess is to set $\mathbf{F} = F_{w0}$. An additional "correction"-step in the Newton's method iteration loop is then applied to force the solution $F_w > \gamma f_w$.

5.2 Convergence

The number of maximum iterations in the Newton's method can be prescribed or it can run until the value of an objective function, *res*, becomes smaller than a predefined tolerance, tol, here the latter is used. An optimal form of the objective function is impossible to define a priori and the tolerance level is often set to some low number that compromises between accuracy and convergence rate. Fucik et al [4] use an objective function based on the difference between values of A in two consecutive iterations. For the study documented in the current article, an objective function based on the residual vector in Eq. (45) is used instead.

After some numerical investigation, it was decided to use $res = \| \mathbf{R}(\mathbf{F})/(10N) \|^2$ and the tolerance level is conveniently defined as $tol = N\varepsilon$ (where ε is a built-in constant in MATLAB, $\varepsilon = 2.22044 \cdot 10^{-16}$).

6 Evaluation of A_D

As stated earlier in section 2.2, A_D is iteratively found for a given S_{w0} such that $F_w(S_{w0}) = F_{w0}$. Therefore, A_D needs to be evaluated in each Newton's method iteration step so that the two variables F_w and A_D converge to a solution. There are several ways to numerically determine A_D. One way is to evaluate the integral in Eq. (35) using the trapezoidal rule. However, a better option, that fits into the pseudospectral framework of solving F_w, is to use Lobatto's integration formula for Chebyshev polynomials of second kind (see section sec. 25.4.41 of Abramowitz and Stegun [1]):

$$\int_a^b \sqrt{(y-a)(b-y)}f(y)dy = \left(\frac{b-a}{2}\right)^2 \sum_{i=1}^{n} w_i f(y_i) + R_n \tag{48}$$

where the abscissas, x_i, the mapped coordinates, y_i, the weights, w_i, and error-term, R_n, are defined, respectively, as:

$$x_i = \cos\left(\frac{i}{n+1}\pi\right) \tag{49}$$

$$y_i = \frac{b+a}{2} + \frac{b-a}{2}x_i \tag{50}$$

$$w_i = \frac{\pi}{n+1}\sin^2\left(\frac{i}{n+1}\pi\right) \tag{51}$$

$$R_n = \frac{\pi}{(2n)!2^{2n+1}} f^{(2n)}(\xi) \tag{52}$$

and $(-1 < \xi < 1)$. Note that in this context, i are the interior nodes, $i = 1, 2, \ldots, n$, and n is the number of interior Chebyshev points; $n = N-2$ (compare with Eq. (36)).

Assuming that R_n is sufficiently small, careful rearrangement of Eq. (48) leads to

$$\int_a^b f(y)dy \approx \frac{\pi}{N-1}\left(\frac{b-a}{2}\right)\sum_{k=1}^{N}\sqrt{1-x_k^2}f(x_k) \tag{53}$$

where $\mathbf{x}_k$ are the Chebyshev points given in Eq. (36). Note that $1-\mathbf{x}_1^2 = 1-\mathbf{x}_N^2 = 0$.

Consideration of Eqs. (35) and (53) reveals that

$$A_D^2 \approx \frac{1}{F_{wi}-F_{w0}}\left\{\frac{\pi}{N-1}\left(\frac{S_{w0}-S_{wi}}{2}\right) \cdot \sum_{k=1}^{N}\sqrt{1-x_k^2}\left[\frac{(S_w-S_{wi})G_D}{F_w-\gamma f_w}\right]_k\right\} \tag{54}$$

where the variables in the last bracket in Eq. (54) (G_D, F_w, f_w and S_{wi}) are evaluated at the Chebyshev points $\mathbf{x}_k$ for $S_w = S_{wk}$.

7 Worked examples using MATLAB

As a demonstration of the new methodology, the worked examples presented in Table 1 of McWhorter and Sunada [8] for unidirectional flow ($\gamma = 1$) are revisited. Here McWhorter and Sunada [8] obtained normalized values of A (called A_n in their manuscript) for a range of different boundary saturations, S_{w0}, and for two values of mobility ratio, $Mo = \mu_w/\mu_n$, $Mo = 2$ and $Mo = 50$.

In addition, similar results for counter-current flow (for $\gamma = 0$ and $\gamma = 0.5$) is demonstrated and presented in Table 2.

The scenarios assume that relative permeability, capillary pressure and saturation are related by relationships previously presented by Parker et al [10] where:

$$k_{rw} = S_e^{1/2}\left[1-(1-S_e^{1/m})^m\right]^2 \tag{55}$$

$$k_{rn} = (1-S_e)^{1/2}(1-S_e^{1/m})^{2m} \tag{56}$$

$$p_{cD} = \frac{p_c}{p_e} = (S_e^{-1/m}-1)^{(1-m)} \tag{57}$$

and m [-] is an empirical constant, set to 0.5, and S_e [-] is an effective saturation. For simplicity, McWhorter and Sunada [8] assume that $S_e = S_w$. Differentiating Eq. (57) with respect to S_w leads to

$$\frac{dp_{cD}}{dS_w} = \frac{p_{cD}(1-m)}{mS_w(S_w^{1/m}-1)} \tag{58}$$

Furthermore, the scenarios assume that the inlet composition is free of non-wetting phase and that the porous media is initially free of wetting-phase, i.e., $\gamma = 1$ and $S_{wi} = 0$. Note that the relationship between A_n (Eq. B4 of McWhorter and Sunada [8]) and A_D is

$$A_D = \frac{A_n}{1-f_{wi}}, \tag{59}$$

but when $f_{wi} = 0$, $A_D = A_n$. Also note that $p_{cD} \to \infty$ when $S_w \to 0$, therefore it is better to set S_{wi} to some suitably small number. Here we set $S_{wi} = 10^{-10}$, hence $A_D \approx A_n$.

The pseudospectral method presented in earlier sections is concisely summarized by the self-contained MATLAB code presented in Fig. 1. The code calculates a value of A_D for a given value of S_{w0} whilst also solving and plotting the associated saturation profile using the Parker et al [10] relationships described above. Note that here, the differentiation matrix is obtained using the `chebdif` function provided by Weideman and Reddy [17].

```
N = 100; % Number of Chebyshev nodes
Swi = 1e-10; % Initial wetting saturation
Sw0 = 0.8; % Injection wetting saturation
Fw0 = 1; % Boundary condition, inlet
Mo = 0.05; % Viscosity ratio, muw/mun
m = 1/2; % Hydraulic Parker property
gam = 1; % Boundary wetting flux/total fluid flux

%Get differentitation matrix
[x,D] = chebdif(N,2);
dxdSw = 2/(Sw0-Swi);
E1 = dxdSw*D(:,:,1);
E2 = dxdSw^2*D(:,:,2);
Sw = (Sw0+Swi)/2+(Sw0-Swi)/2*x;
% Parker et al. (1987) relationships:
krw = sqrt(Sw).*(1-(1-Sw.^(1/m)).^m).^2;
krn = sqrt(1-Sw).*(1-Sw.^(1/m)).^(2*m);
PcD = (Sw.^(-1/m)-1).^(1-m);
dPcDdSw = PcD*(1-m)/m./Sw./(Sw.^(1/m)-1);
fw = 1./(1+Mo*krn./krw);

% Initializing equation system and solving:
GD = fw.*krn*Mo.*dPcDdSw;
i = 2:N-1; % Inner node index
I = eye(N); % Identity matrix
Fwi = gam*fw(N); % Boundary condition, outlet
Fw = Fw0*ones(N,1); % Initial guess
res = 1; tol = N*eps;

while res > tol % Newton's iteration
   fy = (Sw-Swi).*GD./(Fw-gam*fw);
   AD2 = 1/(Fwi-Fw0)*pi/(N-1)/dxdSw*...
        [sqrt(1-x.^2)]'*fy;
   Q = (GD/AD2./(Fw-gam*fw));
   dQ = -GD/AD2./(Fw-gam*fw).^2;
   R = [E2(i,:)*Fw-I(i,:)*Q;Fw(N)-Fwi;...
        Fw(1)-Fw0];
   dR = [E2(i,:)-I(i,:)*diag(dQ);I(N,:);I(1,:)];
   Fw = max(gam*fw+tol/2,Fw-dR\R);
   res = norm(R/10/N).^2;
end
plot(E1*Fw,Sw)
```

Fig. 1 MATLAB code to solve two-phase flow with capillary pressure. This particular code snippet will give the plot for unidirectional flow ($\gamma = 1$) for $S_{w0} = 0.8$ and $Mo = 0.05$ in Fig. 2. To create the differentiation matrix the function `chebdif.m` from Weideman and Reddy [17] is used. (Alternatively `cheb.m` from Trefethen [16] can be used.)

Table 1 Calculated values of A_D for unidirectional flow ($\gamma = 1$) for various injection wetting saturations, S_{w0}, at two viscosity ratios, $Mo = 2$ and $Mo = 50$. The values for A_D reported by (reported as A_n by McWhorter and Sunada [8]) are given in brackets. The number of iterations required by Newton's method is also given.

$Mo = 2$			$Mo = 50$		
S_{w0}	A_D	Iter	S_{w0}	A_D	Iter
0.25	0.011 (0.011)	8	0.25	0.011 (0.011)	8
0.5	0.058 (0.058)	7	0.5	0.058 (0.058)	7
0.7	0.138 (0.138)	7	0.7	0.137 (0.138)	6
0.9	0.308 (0.308)	6	0.9	0.307 (0.307)	6
0.95	0.395 (0.395)	7	0.95	0.390 (0.392)	6
0.99	0.533 (0.534)	10	0.99	0.516 (0.516)	6
0.9995	0.661 (0.703)	25	0.9995	0.602 (0.629)	6
0.9999	0.695 (0.850)	42	0.9999	0.615 (0.709)	7

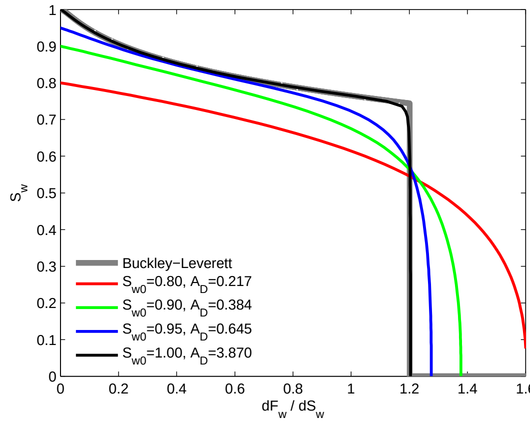

Fig. 2 Saturation distributions for various values of S_{w0} using the same scenario as described for Table 1, but with a lower viscosity ratio, $Mo = 0.05$. For comparison purposes, the Buckley-Leverett solution is plotted alongside as a thicker grey line (note that $S_{w0} = 1.00$ is actually $S_{w0} = 0.999999$). The corresponding fractional flow ratios F_w and the fractional flow function f_w are given in Fig. 3.

By comparing values for A_D obtained using the pseudospectral method and the values reported by McWhorter and Sunada [8] (see Table 1), it can be seen that the results are in very good agreement for injection wetting saturations up to $S_{w0} = 0.99$. For higher saturation values it is observed, as reported by McWhorter and Sunada [8], that A is quite sensitive to changes in S_{w0} and deviations are seen in the results. This is believed to be due to the different solution procedures used here and by McWhorter and Sunada [8].

A numerical test using the trapezoidal rule (as opposed to Lobatto's integration formula) for integration gives comparable values to those obtained by McWhorter and Sunada [8], using $N = 33$ and $N = 25$ for the viscosity ratios $Mo = 2$ and $Mo = 50$, respectively. For $S_{w0} = 0.9 - 0.9999$ the values for A_D were [0.309 0.396 0.538 0.706 0.851] and [0.308 0.393 0.523 0.638 0.708] for $Mo = 2$ and $Mo = 50$, respectively. The values are very close to the values reported by McWhorter and Sunada [8]. However, by refining the discretization (by increasing N) the values again approach those using Lobatto's integration formula given in Table 1.

From Eq. (16), as capillary pressure becomes negligible (e.g. by setting $\gamma = 1$ and increasing A_D) the value of F_w approaches the Buckley-Leverett solution. From Table 1 it can be seen that as S_{w0} increases, so does A_D (and hence q_t). To see how this solution approaches the Buckley-Leverett solution, various saturation curves for $S_{w0} \to 1$ are plotted in Fig. 2. Note that a viscosity ratio of $Mo = 0.05$ was used to obtain a more distinct two-phase region. Following Fucik et al [4], Buckley-Leverett solution is plotted alongside pseudospectral results as a thicker grey line. Fig. 2 confirms that the pseudospectral method is capable of solving the McWhorter and Sunada [8] equation approaching the Buckley-Leverett solution.

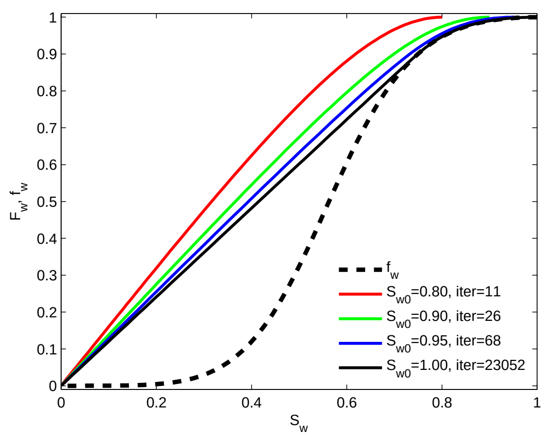

Fig. 3 The fractional flow ratios F_w for the various saturation curves given in Fig. 2 and the fractional flow function f_w. The number of Newton's method iterations required are given in the legend. Note that $S_{w0} = 1.00$ is actually $S_{w0} = 0.999999$.

Counter-current flow is controlled by the parameter γ. Fig. 4 shows the saturation profiles for various γ: $\gamma = 0$, 0.9, 0.99, 0.9999 and 1, together with the corresponding Buckley-Leverett solution. The corresponding fractional flow ratios, F_w, and the fractional flow function, f_w, are shown in Fig. 5.

Table 2 Calculated values of A_D for counter-current flow ($\gamma = 0$ and $\gamma = 0.5$) for various injection wetting saturations, S_{w0}, and viscosity ratio, $Mo = 2$. The number of iterations required by Newton's method is also given.

$\gamma = 0$			$\gamma = 0.5$		
S_{w0}	A_D	Iter	S_{w0}	A_D	Iter
0.25	0.011	8	0.25	0.011	8
0.5	0.057	7	0.5	0.057	7
0.7	0.134	7	0.7	0.136	7
0.9	0.248	6	0.9	0.269	6
0.95	0.267	7	0.95	0.299	7
0.99	0.274	7	0.99	0.311	7
0.9995	0.275	7	0.9995	0.312	7
0.9999	0.275	7	0.9999	0.312	7

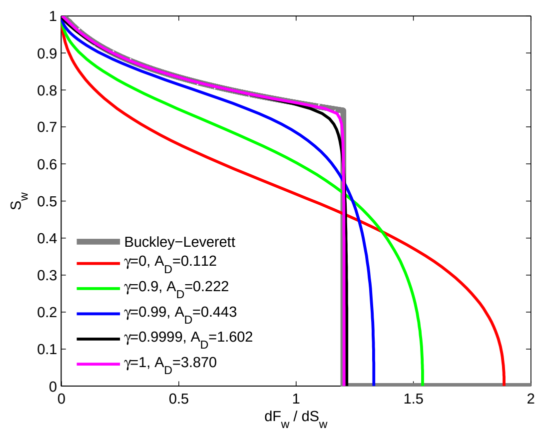

Fig. 4 Saturation profiles for various values of γ for $S_{w0} = 0.999999$ and viscosity ratio, $Mo = 0.05$. For comparison purposes, the Buckley-Leverett solution is plotted alongside as a thicker grey line.

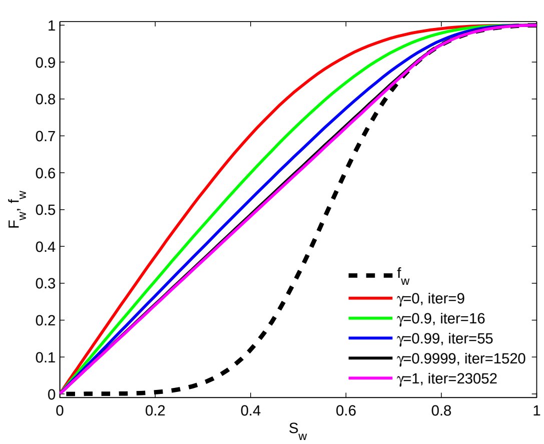

Fig. 5 The fractional flow ratios F_w for the various saturation curves given in Fig. 4 and the fractional flow function f_w. The number of Newton's method iterations required are given in the legend. Injection saturation is $S_{w0} = 0.999999$.

In terms of performance, the number of iterations used in the various simulations are reported in Table 2 and Fig. 5. The number of iterations required to achieve convergence depends not only on the number of Chebyshev nodes N and convergence criterion that is used, but also key parameters such as viscosity ratio and hydraulic relations like the relative permeability functions and capillary pressure function. It can be seen, for instance, by comparing the number of iterations in Table 1 and Fig. 3 that by lowering the viscosity ratio Mo from 2 to 0.05, the number of iterations increase from 7 to 68 for $S_{w0} = 0.95$. Although Fucik et al [4] use a different convergence criterion, it is interesting to note, from their Table 5 for setup 3, method B (which is the scenario closest to that studied by McWhorter and Sunada [8], see Table 1), that the number of iterations required were 38, 99, 1493, 121891 and 7067090 for $S_{w0} = 0.5, 0.7, 0.9, 0.99$ and 0.999, respectively.

8 Summary and conclusion

An alternative approach for solving the McWhorter-Sunada integral equation for immiscible and incompressible unidirectional and counter-current two-phase flow through a homogeneous, one-dimensional porous media with capillary pressure, has been presented. A normalized and self-similar governing equation has been solved using a Chebyshev spectral collocation (pseudospectral) method and compared to its original integral equation solution. Both methods compare favorably for unidirectional flow and saturations up to $S_{w0} = 0.99$. For $S_{w0} > 0.99$, deviation between the two methods is noticed. It could be argued that the discrepancy is due to the use of different solution schemes. However, the results obtained using the pseudospectral method should be more accurate due to the use of Nth-order (100th-order in this case) polynomials associated with the Chebyshev differentiation matrix. The pseudospectral method is also found to be capable of solving for boundary wetting saturations approaching 1 (during imbibition) and also for elevated injection rate where the saturation profiles approach that of the Buckley-Leverett solution (when the capillary pressure effect becomes negligible). The new methodology is concisely summarized by a self-contained MATLAB code, which should greatly assist use of the McWhorter-Sunada equation in the future.

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