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Self-similar Profiles for Capillary Diffusion Driven Flow in Heterogeneous Porous Media

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Abstract

In this paper we consider the process of one-dimensional redistribution of two immiscible and incompressible fluids in a heterogeneous porous medium. We treat in detail the special case in which the initial saturation as well as the properties of the porous medium have a single coinciding discontinuity. Then the time-dependent saturation profile is of self-similar form, i.e. depends only on x/\sqrt{t} . This self-similar profile can be used to validate numerical algorithms describing two-phase flow in porous media with discontinuous heterogeneities. We discuss the construction of the similarity solution, in which we give special attention to the matching conditions at the interface where the medium properties are discontinuous. We also outline a numerical procedure to obtain the similarity solution and we provide applications in terms of the Brooks-Corey and the Van Genuchten model.

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1 Introduction

Numerical models are effective tools to study two-phase flow in heterogeneous porous media. These models need to be verified and validated, however. For

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the purpose of verification of the underlying mathematical model, laboratory experiments and field tests are indispensable. The validation of the numerical model is often established by comparing the numerical solutions to analytical solutions of specific test problems.

A well-known test problem is the Buckley-Leverett problem [5]. The solution of this problem describes the flow of two phases in a homogeneous porous medium in the absence of capillarity. When capillary forces are present, analytical solutions are known for some specific cases only. For instance, Sunada & McWorther [8] incorporated the capillary pressure in their formulation, and derived a similarity solution for the one-dimensional displacement of a nonwetting phase with a total flow rate varying inversely proportional to the square root of time. They also derived a similarity solution for two-dimensional radial flow with a constant total flow rate. Similarity solutions in the case that there is no convection, but only redistribution of the two phases, were found by Philip [9],[10], Van Duijn & Peletier [13] and Van Duijn & Floris [11] (non-Newtonian fluids). All these papers are dealing with homogeneous porous media.

To our knowledge, not so many exact solutions are known for porous media that contain heterogeneities. Yortsos & Chang [15] have obtained steady-state solutions for a heterogeneous medium, in which two regions of constant permeability are connected by a linear transition. Van Duijn, Molenaar & De Neef [12] derived steady-state solutions for a discontinuous heterogeneity. No time-dependent exact solutions for two-phase flow through porous media with a heterogeneity were found in the literature.

In this paper we present a method to construct a time-dependent solution of self-similar form describing the one-dimensional redistribution of two immiscible and incompressible phases in a heterogeneous porous medium. The redistribution of the phases is caused by capillary forces. The porous medium consists of two homogeneous media of infinite extent which are joined at the origin, so that the permeability and the porosity have a jump discontinuity there, and are constant elsewhere. We will show that this problem possesses a similarity solution if one medium is initially saturated by the wetting phase, and the other by the nonwetting phase.

The interface conditions at surfaces where the permeability or porosity are discontinuous play a crucial role in the construction of the solution. The two conditions that need to be imposed have been derived by Van Duijn, Molenaar & De Neef [12]. One condition is that the flux must be continuous across the interface. The other, which is called the extended pressure condition, is a nonlinear relation between the wetting phase saturation at the left- and right-hand side of the discontinuity. It strongly depends on the qualitative behaviour of the capillary pressure.

One aspect in particular plays an important role: the entry pressure. The entry pressure, also known as the displacement pressure or threshold pressure, is the minimum pressure that is needed for a nonwetting fluid to enter a

medium that is initially saturated by wetting fluid. When the entry pressure is positive, it may happen that the capillary pressure is not continuous across the interface. Nonetheless, we shall show that the interface conditions still lead to a unique similarity solution.

The diffusion problem discussed here resembles in many respects the onedimensional hysteresis problem studied by Philip [10]. In that paper he considers the redistribution of water in an unsaturated soil with different capillary pressure curves on the left- and right-hand side of the origin: a drying curve on one side, a wetting curve on the other side. By a so-called flux-concentration method, Philip obtains approximate solutions for this problem. The solutions in his case always have continuous capillary pressure, since the drying and the wetting curve form a closed loop (the hysteresis loop) with zero entry pressure. In this work we give the procedure to obtain solutions without approximations, we outline a numerical method to approximate the exact solution, and we allow the solutions to have discontinuous capillary pressure.

This paper is organised as follows. In Section 2 we present the mathematical model describing the redistribution of two immiscible phases in a porous medium. Further we explain the interface conditions needed at a discontinuity in the permeability or porosity.

In Section 3 we use a similarity transformation to transform the partial differential equation into an ordinary differential equation. For this latter equation we shall explain how the solution can be constructed. We give a criterion to determine whether the solution has discontinuous capillary pressure or not. This can be checked before the actual construction of the solution. The technical details of the mathematical justification are presented elsewhere [6]. Furthermore we provide a numerical method and we discuss the qualitative behaviour of the solution.

In Section 4 we give two illustrative examples. We consider similarity solutions for two different models of the capillary-hydraulic properties of the porous medium: the Brooks-Corey model [4] and the Van Genuchten model [14]. Since a Brooks-Corey type of porous medium has a positive entry pressure, solutions may occur with discontinuous capillary pressure. We provide an example of such a solution.

2 Mathematical Model

In this section we give the mathematical formulation of the redistribution of two immiscible and incompressible phases in a saturated and heterogeneous porous medium. We assume that the heterogeneity of the porous medium, i.e. porosity ϕ and permeability k, varies in one direction only, say the x-direction. Further we assume that the fluid flow is one-dimensional in that direction. We characterise the phases by their reduced saturations: S_w (saturation of the

wetting fluid) and S_n (saturation of the nonwetting fluid), with $0 \le S_w$, $S_n \le 1$. Since the porous medium is assumed to be saturated we have

$$S_w + S_n = 1. (1)$$

The equations governing the flow of each phase are (e.g. Bear [3]) the fluid-balance equations

$$\phi \frac{\partial S_i}{\partial t} + \frac{\partial q_i}{\partial x} = 0, \quad i = w, n, \tag{2}$$

and Darcy's law,

$$q_i = -\lambda_i \frac{\partial p_i}{\partial x}, \quad i = w, n.$$
 (3)

Here q_i , λ_i and p_i (i = w, n) denote the specific discharge, the mobility and the pressure of the wetting and nonwetting phase. In writing equation (3) we assumed that the flow is horizontal, so that gravitational forces in the direction of the flow are absent. The mobility of each phase is given by

$$\lambda_i = \frac{k(x)k_{ri}(S_w)}{\mu_i}, \quad i = w, n, \tag{4}$$

where k is the absolute permeability of the porous medium, and k_{ri} and μ_i the relative permeability and viscosity of phase i.

Because of interfacial tension on the microscopic pore level, the pressures of the wetting and the nonwetting fluid differ. This pressure difference, which is called the capillary pressure p_c , obeys the Leverett-relationship (cf. [7])

$$p_n - p_w = p_c(x, S_w) = \sigma \sqrt{\frac{\phi(x)}{k(x)}} J(S_w), \tag{5}$$

where σ is the interfacial tension, and J the Leverett function.

Equations (1)-(5) can be combined into one equation for the saturation of the wetting phase S_w . When we add the equations (2) for i = w and i = n, and use (1), we find that the total flow rate q, defined by

$$q = q_w + q_n, (6)$$

is constant in space. Using this observation and combining equations (1)–(6) we obtain a non-linear convection-diffusion equation for the water saturation S_w . Because we want to describe the *redistribution* of the phases only, we set q = 0, which results in a nonlinear diffusion problem for S_w .

To put the equation into an appropriate dimensionless form, we choose characteristic quantities T (time), L (length), k^* (permeability), and ϕ^* (porosity), and redefine the variables according to

$$t := \frac{t}{T}, \quad x := \frac{x}{L}, \quad k := \frac{k}{k^*}, \quad \phi := \frac{\phi}{\phi^*}. \tag{7}$$

This yields

$$\phi \frac{\partial u}{\partial t} + \frac{\partial}{\partial x} \left(k \bar{\lambda}(u) \frac{\partial}{\partial x} \left(\sqrt{\phi/k} J(u) \right) \right) = 0, \tag{8}$$

where u = u(x,t) denotes the reduced saturation of the wetting fluid. Further

$$\bar{\lambda}(u) = N_c \frac{k_{rw}(u)k_{rn}(u)}{k_{rw}(u) + k_{rn}(u)/M},$$

with

$$N_c = \frac{\sigma \sqrt{\phi^* k^*}}{\mu_n \phi^* (L/T)}$$
 and $M = \frac{\mu_n}{\mu_w}$.

The positive numbers N_c and M are called the capillary number and the mobility ratio.

We assume throughout this work that the relative permeabilities k_{rw} and k_{rn} are continuous on [0,1], and that J is continuous on [0,1] and continuously differentiable on (0,1). Further we assume that they satisfy

- k_{rw} is strictly increasing such that $k_{rw}(0) = 0$ and $k_{rw}(1) = 1$;
- k_{rn} is strictly decreasing such that $k_{rn}(0) = 1$ and $k_{rn}(1) = 0$;
- $\lim_{u\downarrow 0} J(u) = \infty$, J' < 0 on (0,1) and $J(1) \ge 0$.

The conditions $k_{rw}(1)$, $k_{rn}(0) = 1$ can be relaxed to allow for $k_{rw}(1)$, $k_{rn}(0) \neq 1$. This would only affect the mobility ratio M and the capillary number N_c .

Because J'(u) may be unbounded as u tends to zero or one, the diffusivity $-J'(u)\bar{\lambda}(u)$ can be unbounded there as well. To avoid this we assume in addition that $J'(u)\bar{\lambda}(u)$ is continuous on [0,1], and hence bounded. This condition is satisfied for most of the functions J and $\bar{\lambda}$ found in the literature, e.g. Brooks-Corey and Van Genuchten functions (cf. Section 4).

2.1 Medium with a single discontinuity

In order to construct similarity solutions later on, we need to restrict ourselves to a porous medium of which the permeability and porosity change abruptly at some point, say at x = 0, and are constant elsewhere. The permeability and the porosity then satisfy

$$k(x) = \begin{cases} k_l & x < 0, \\ k_r & x > 0, \end{cases} \quad \text{and} \quad \phi(x) = \begin{cases} \phi_l & x < 0, \\ \phi_r & x > 0. \end{cases}$$
 (9)

For such a medium we obtain the equations

$$\frac{\partial u}{\partial t} = h_l \frac{\partial}{\partial x} \left(D(u) \frac{\partial u}{\partial x} \right) \quad \text{for } x < 0, \ t > 0,$$
 (10)

$$\frac{\partial u}{\partial t} = h_r \frac{\partial}{\partial x} \left(D(u) \frac{\partial u}{\partial x} \right) \quad \text{for } x > 0, \ t > 0,$$
 (11)

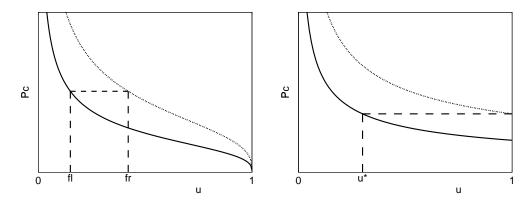


Figure 1: Capillary pressure p_c as a function of the reduced water saturation u. The dashed curves correspond to fine, and the solid ones to coarse materials. The entry pressure at u = 1 is either zero (left) or positive (right).

where

$$D(u) = -J'(u)\bar{\lambda}(u), \tag{12}$$

and where we introduced for convenience

$$h_l = (k_l/\phi_l)^{1/2}$$
 and $h_r = (k_r/\phi_r)^{1/2}$. (13)

The conditions imposed on k_{rw} , k_{rn} and J imply that D(u) is nonnegative and continuous on [0,1], and D(u) > 0 on (0,1).

At x = 0 where k and ϕ have a discontinuity, the equations do not hold. At this point we need to impose two interface conditions for all t > 0. The first condition is continuity of the flux,

$$\lim_{x \uparrow 0} \left(-\phi_l h_l D(u) \frac{\partial u}{\partial x} \right) = \lim_{x \downarrow 0} \left(-\phi_r h_r D(u) \frac{\partial u}{\partial x} \right). \tag{14}$$

The second interface condition is an extension of a continuity condition for the capillary pressure. This extended pressure condition, which is derived by Van Duijn, Molenaar and De Neef [12], is explained as follows.

The media to the left and right of x = 0 have different values of $h := (k/\phi)^{1/2}$. As a result they have different capillary pressure curves, which follows directly from the Leverett-relationship (5). If for example $h_l > h_r$, i.e. coarse material to the left and fine material to the right of x = 0, then the capillary pressure curve corresponding to the fine material lies above the curve corresponding to the coarse material (cf. Figure 1). We distinguish capillary pressure curves for which the entry pressure is zero, Figure 1 (left), and curves for which it is positive, Figure 1 (right).

If the entry pressure is zero, then to every saturation on one side of the interface, there corresponds a saturation on the other side so that the capillary

pressure is continuous (cf. Figure 1 (left)). In this case the second interface condition is simply continuity of capillary pressure, which is expressed by

$$\frac{J(u_r)}{h_r} = \frac{J(u_l)}{h_l},\tag{15}$$

where u_r and u_l denote the right and left limit value of u at x = 0. Condition (15) is used in the analysis by Philip [10].

If, however, the entry pressure is positive, we see from Figure 1 (right) that there is a threshold saturation u^* such that continuity of capillary pressure cannot be established unless the wetting phase saturation on the side corresponding to the lower curve is less than or equal to u^* . The threshold saturation u^* is determined by (assuming $h_l > h_r$)

$$\frac{J(u^*)}{h_l} = \frac{J(1)}{h_r}. (16)$$

If the wetting phase saturation on the side of the interface that corresponds to the lower curve is greater than u^* , then the saturation on the other side is equal to one, and the capillary pressure across the interface is discontinuous. The extended pressure condition is then given by (assuming $h_l > h_r$)

$$\begin{cases}
\frac{J(u_r)}{h_r} = \frac{J(u_l)}{h_l} & \text{if } u_l \le u^*, \\
u_r = 1 & \text{if } u^* < u_l \le 1.
\end{cases}$$
(17)

If $h_l \leq h_r$ then the second interface condition is given by (17) with the subscripts l and r reversed; the threshold saturation u^* follows then from (16) with h_l and h_r reversed.

A typical example of a porous medium with zero entry pressure is given by the Van Genuchten model [14], one with positive entry pressure by the Brooks-Corey model [4]. We shall discuss both these models, and the corresponding solutions, in Section 4.

3 Similarity solutions

In this section we study the equations (10)–(11) subject to the initial condition

$$u(x,0) = \begin{cases} 1 & \text{if } x < 0, \\ 0 & \text{if } x > 0. \end{cases}$$
 (18)

The resulting problem admits solutions of self-similar form. If we set

$$u(x,t) = f(\eta), \text{ with } \eta = \frac{x}{\sqrt{t}},$$
 (19)

we obtain for f the ordinary differential equations

$$\frac{1}{2}\eta f' + h_l (D(f)f')' = 0 \text{ for } \eta < 0, \tag{20}$$

$$\frac{1}{2}\eta f' + h_r \left(D(f)f' \right)' = 0 \text{ for } \eta > 0.$$
 (21)

Here the primes denote differentiation with respect to η . The initial condition for u yields the boundary conditions

$$f(-\infty) = 1$$
 and $f(\infty) = 0$. (22)

At $\eta = 0$, the solution has to satisfy the flux continuity condition

$$\lim_{\eta \uparrow 0} \left(-\phi_l h_l D(f) f' \right) = \lim_{\eta \downarrow 0} \left(-\phi_r h_r D(f) f' \right) \tag{23}$$

and the extended pressure condition (17) with u_r and u_l replaced by $f_r = \lim_{\eta \downarrow 0} f(\eta)$ and $f_l = \lim_{\eta \uparrow 0} f(\eta)$.

3.1 Construction of the solution

To construct the similarity solution, we first solve (20), (21) and (22) and then match the corresponding solutions at $\eta = 0$ so that the interface conditions (17) and (23) are satisfied.

Thus we start with the subproblems

$$P_{-} \begin{cases} \frac{1}{2} \eta f' + h_{l} (D(f)f')' = 0, & -\infty < \eta < 0, \\ f(-\infty) = 1, & f(0) = f_{l}, \end{cases}$$

and

$$P_{+} \begin{cases} \frac{1}{2} \eta f' + h_{r} (D(f)f')' = 0, & 0 < \eta < \infty, \\ f(0) = f_{r}, & f(\infty) = 0, \end{cases}$$

where $0 \le f_l, f_r \le 1$ have to be determined from the interface conditions.

It is well-known (e.g. De Neef [6] and Van Duijn & Peletier [13]) that Problem P_- has a unique solution $f_- = f_-(\eta)$ for every $f_l \in [0,1]$. If $f_l = 1$ then $f_-(\eta) = 1$ for all $\eta \leq 0$; if $f_l < 1$ then there exists a number $-\infty \leq a_- < 0$ such that

$$f_{-}(\eta) \begin{cases} = 1 & \text{for } \eta \leq a_{-}, \\ < 1 \text{ and strictly decreasing} & \text{for } a_{-} < \eta < 0. \end{cases}$$

The behaviour of the diffusion coefficient near f=1 determines whether $a_-=-\infty$ or $a_->-\infty$. The precise condition is given in Section 3.2.

Similarly, Problem P_+ has a unique solution $f_+ = f_+(\eta)$ for every $f_r \in [0, 1]$. If $f_r = 0$ then $f_+(\eta) = 0$ for all $\eta \geq 0$; if $f_r > 0$ then there exists a number $0 < a_+ \leq \infty$ such that

$$f_{+}(\eta)$$
 $\begin{cases} > 0 \text{ and strictly decreasing} & \text{for } 0 < \eta < a_{+}, \\ = 0 & \text{for } \eta \geq a_{+}. \end{cases}$

Here the behaviour of the diffusion coefficient near f = 0 determines whether $a_+ = \infty$ or $a_+ < \infty$. For the precise condition we refer to Section 3.2.

To apply the interface conditions we need to know the fluxes at $\eta = 0$. Let

$$F_l := -\phi_l h_l D(f_l) f'_-(0)$$

and

$$F_r := -\phi_r h_r D(f_r) f'_+(0).$$

For every value of $f_l \in [0,1]$, which determines the solution f_- of Problem P_- , a unique F_l results. We denote this dependence by writing $F_l = F_l(f_l)$. This function is continuous and decreasing in $f_l \in [0,1]$ such that $F_l(1) = 0$. An analytic proof of these statements is given by Van Duijn & Peletier [13]; a computational result is shown in Figure 2, where the flux function F_l is given for the Brooks-Corey and the Van Genuchten model.

In a similar fashion F_r can be considered as a function of f_r . This function, which is continuous and increasing in $f_r \in [0,1]$ with $F_r(0) = 0$, is shown in Figure 2.

Having discussed these preliminary results, we can now outline the matching procedure.

3.1.1 Existence of a unique pair (f_l, f_r)

We consider in detail the case $h_l > h_r$. In Figure 2 the graphs of the capillary pressure and the fluxes are shown, both as functions of the saturation at each side of the origin. Note that here the lower capillary pressure curves correspond to the left-hand side of the origin, the upper curves to the right-hand side. The fluxes were obtained by numerically solving transformed versions of Problems P_- and P_+ for different f_l and f_r . The details of the transformation and computation are given in Section 3.1.2. We treat the cases with and without entry pressure separately.

Zero entry pressure

If the entry pressure is zero, then the saturations at the origin have to satisfy condition (15), reflecting continuity of the capillary pressure. Since the capillary pressure functions are strictly decreasing, it follows from continuity of the capillary pressure that the right saturation depends monotonically on

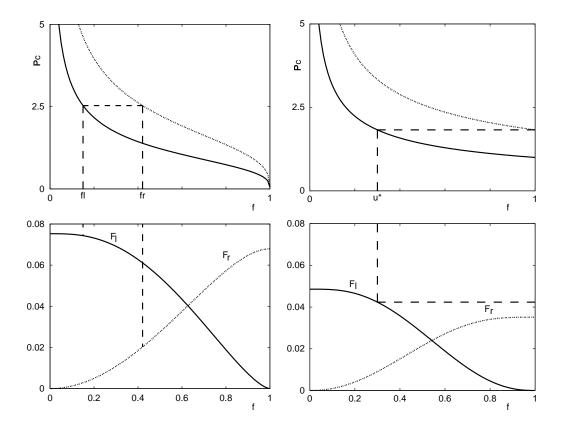


Figure 2: Capillary pressure (upper figures) and flux (lower figures) as a function of the saturation. The solid curves correspond to the left, the dashed curves to the right side of the origin. The left figures are obtained for the Van Genuchten model (zero entry pressure), the right figures for the Brooks-Corey model (positive entry pressure). The data used for the computation of the fluxes are given in Table 1.

the left saturation (cf. Figure 2 (left)): for instance, when we increase the left saturation f_l , then the right saturation f_r increases as well. Furthermore, for increasing f_l , the left flux F_l decreases while the corresponding right flux increases.

Now using continuity and monotonicity of the graphs in Figure 2 (left), we find, for f_l increasing from zero, a unique pair (f_l, f_r) such that both pressure and flux are equal. The continuity of the fluxes combined with $F_l(0) > F_r(0)$ and $F_l(1) < F_r(1)$ yields the existence of such a pair. The monotonicity of the fluxes implies the uniqueness.

Positive entry pressure

If the entry pressure is positive, as in Figure 2 (right), then the situation is different in the sense that now the saturations at the discontinuity are related to each other through the extended pressure condition (17). Increasing the left saturation f_l , we see that the right saturation increases only if $f_l \leq u^*$, but is constant $(f_r = 1)$ if $f_l > u^*$. Moreover, for increasing f_l , the left flux F_l decreases while the corresponding right flux F_r increases only if $f_l \leq u^*$, but is constant $(F_r = F_r(1))$ if $f_l > u^*$.

So, if $F_l(u^*) > F_r(1)$, then f_l must be greater than u^* in order to have continuity of the flux. In that case $f_r = 1$, and $F_r = F_r(1)$. Since $F_l(f_l)$ is a strictly decreasing function of f_l with $F_l(1) = 0$, it follows that there is a unique f_l such that continuity of the flux is satisfied. Note that the capillary pressure is discontinuous in this case.

If $F_l(u^*) \leq F_r(1)$, then it is necessary that $f_l \leq u^*$ in order to have continuity of flux. Consequently the capillary pressure is continuous, and again as in the case of zero entry pressure, there is a unique pair (f_l, f_r) , such that the interface conditions are satisfied.

Remark. The case $h_l \leq h_r$ can be treated in a similar manner. In that case too, the pair (f_l, f_r) is uniquely determined. However now the capillary pressure is always continuous, since f_l must be less than one in order to have a positive flux F_l , and therefore $f_r < u^*$.

3.1.2 Computation of the solution

To obtain a solution, first determine the pair (f_l, f_r) that satisfies the interface conditions, and then use these values to solve Problems P_- and P_+ . It is not necessary to solve these problems directly: we can obtain their solutions by the method that will be used to compute the fluxes F_l and F_r .

We first explain how to obtain the pair (f_l, f_r) . For the time being, let us assume that the functions $F_l(f_l)$ and $F_r(f_r)$ are known: later on we discuss how they can be approximated numerically. We distinguish between the cases $h_l > h_r$ (capillary pressure possibly discontinuous) and $h_l \leq h_r$ (capillary pressure continuous).

If $h_l > h_r$ we first have to check whether the capillary pressure is continuous. Determine to that purpose $F_l(u^*)$ and $F_r(1)$. If $F_l(u^*) > F_r(1)$, then the capillary pressure is discontinuous, and hence $f_r = 1$. In that case we have to find the root $f_l \in (u^*, 1)$ of

$$F_l(f_l) = F_r(1). (24)$$

If $F_l(u^*) \leq F_r(1)$, then the capillary pressure is continuous, and hence $f_l \leq u^*$. In that case determine f_r as a function of f_l using continuity of capillary pressure. Then find the root $f_l \leq u^*$ that solves the equation

$$F_l(f_l) = F_r(f_r(f_l)). \tag{25}$$

If $h_l \leq h_r$, then the capillary pressure is continuous and we proceed as above: determine f_r as a function of f_l using continuity of capillary pressure, and find the root $f_l \in (0,1)$ that solves (25). To find the root of (24) or (25) we used the bisection method.

Crucial in the construction are the flux functions $F_l(f_l)$ and $F_r(f_r)$. Of course it is not necessary to determine the entire graphs of F_l and F_r . The functions F_l and F_r only have to be evaluated at the iteration points resulting from the algorithm that is used to find the root of (24) or (25). We discuss below how $F_r(f_r)$, with $0 \le f_r \le 1$, can be approximated numerically. The function $F_l(f_l)$ is approximated in an entirely analogous way. Therefore those details are omitted.

To determine the right flux $F_r(f_r)$ we need to solve Problem P_+ and compute the flux at $\eta = 0$. The complication here is the boundary condition $f_+(\infty) = 0$ which is not always easy to verify. Fortunately there is a more direct way to obtain the flux-saturation relation at $\eta = 0$. The idea is to transform equation (21) into a differential equation for the flux with the saturation as independent variable (see e.g. Van Duijn & Floris [11]). Since f_+ is strictly decreasing on $(0, a_+)$ we can invert

$$f_+ = f_+(\eta)$$
 for $0 \le \eta \le a_+$,

to obtain

$$\eta = \sigma_+(f) \quad \text{for} \quad 0 \le f \le f_r,$$

where σ_+ is the inverse of f_+ with $\sigma_+(0) = a_+$ and $\sigma_+(f_r) = 0$. Next consider the scaled flux (up to the porosity) as a function of saturation, i.e.

$$y(f) := -h_r D(f) f'_+(\sigma_+(f)) \quad \text{for } 0 \le f \le f_r.$$
 (26)

Note that y(f) > 0 for $0 < f < f_r$, because f_+ is monotonically decreasing. Using equation (21), one easily verifies that

$$\frac{dy}{df}(f) = \frac{1}{2}\sigma_{+}(f) \quad \text{for } 0 < f < f_r, \tag{27}$$

and

$$y \frac{d^2 y}{df^2} = -\frac{1}{2} h_r D(f) \quad \text{for } 0 < f < f_r.$$
 (28)

Since the flux vanishes whenever the saturation vanishes we also have y(0) = 0. Thus for given $f_r \in [0, 1]$, we want to solve the boundary value problem

(BVP)
$$\begin{cases} y \frac{d^2 y}{df^2} = -\frac{1}{2} h_r D(f) & \text{for } 0 < f < f_r, \\ \frac{dy}{df} (f_r) = 0, \quad y(0) = 0, \end{cases}$$

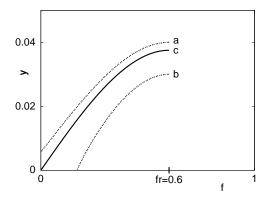


Figure 3: Shooting procedure to solve Problem (BVP): (a) $y_r = 0.04$, (b) $y_r = 0.03$, and (c) $y_r = 0.03752$, required y_r limit value. The Van Genuchten model is used here, with data taken from Table 1.

such that y > 0 on $(0, f_r)$. Having established the solution y = y(f), we know the flux at $\eta = 0$ through the relation

$$F_r(f_r) = \phi_r y(f_r). \tag{29}$$

Problem (BVP) is solved by a shooting technique. Instead of the boundary conditions of Problem (BVP), we consider the initial conditions

$$\begin{cases} y(f_r) = y_r & (> 0, \text{ a priori unknown}), \\ \frac{dy}{df}(f_r) = 0, \end{cases}$$

and solve the differential equation of Problem (BVP) with a Runge-Kutta method in the interval $0 < f < f_r$. The parameter y_r is chosen such that the boundary condition y(0) = 0 is satisfied. We used the bisection method to obtain fast convergence to the required value of y_r . The shooting procedure is illustrated in Figure 3.

The method to compute y(f) can be conveniently employed to determine the approximate solution f_+ of Problem P_+ . In the Runge-Kutta procedure, the second-order differential equation in y is rewritten into a system of firstorder differential equations in the dependent variables y and dy/df. Now, from (27) we have

$$\frac{dy}{df}(f_{+}(\eta)) = \frac{1}{2}\eta \quad \text{for } 0 < \eta < a_{+},$$
(30)

where a_{+} is given by

$$\frac{dy}{df}(0^{+}) = \frac{1}{2}a_{+} \quad (\leq \infty). \tag{31}$$

Hence, using equation (30), the algorithm directly gives for every value of f the corresponding value of η . This yields the approximate solution of Problem P_+ , as illustrated in Figure 4.

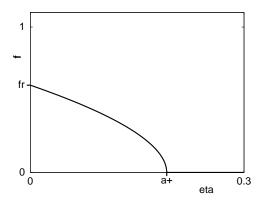


Figure 4: Solution of Problem P_+ with $f_r = 0.6$, obtained by using (30) with y = y(f) from Figure 3.

3.2 Structure of the solution

From what we learned so far we deduce that the self-similar form of the solution, $u(x,t)=f(\eta)$ with $\eta=x/\sqrt{t}$, has a discontinuity at the origin x=0 $(\eta=0)$, where the initial saturation as well as the properties of the porous medium are discontinuous. Moreover, there exist numbers $-\infty \leq a_l < 0 < a_r \leq \infty$ such that

$$f(\eta) \begin{cases} = 1 & \text{for } \eta \leq a_l, \\ \in (0,1) \text{ and strictly decreasing} & \text{for } a_l < \eta < 0 \text{ and } 0 < \eta < a_r, \\ = 0 & \text{for } \eta \geq a_r. \end{cases}$$

Let us assume for the moment that the numbers a_l and a_r are finite. They characterise moving or free boundaries in the x, t-plane, given by

$$x_l(t) = a_l \sqrt{t}$$
 and $x_r(t) = a_r \sqrt{t}$, for $t \ge 0$. (32)

This implies that the saturation as a function of position and time satisfies

$$u(x,t) \begin{cases} = 1 & \text{for } x \le x_l(t), \ t \ge 0 \\ \in (0,1) & \text{for } x_l(t) < x < 0 \text{ and } 0 < x < x_r(t), \ t > 0, \\ = 0 & \text{for } x \ge x_r(t), \ t \ge 0. \end{cases}$$

Moreover

$$\lim_{x \uparrow 0} u(x,t) = f_l \quad \text{and} \quad \lim_{x \downarrow 0} u(x,t) = f_r \quad \text{for all } t > 0.$$

In the mathematics literature, precise results are known concerning the finiteness of a_l and a_r , and concerning the behaviour of the similarity solution near these points, e.g. Atkinson & Peletier [1], [2] or Van Duijn & Floris [11]. These results are related to the behaviour of the diffusion coefficient near f = 1 and near f = 0. Following [1], we find that

$$a_l > -\infty$$
 if and only if
$$\int_0^1 \frac{D(s)}{1-s} ds < \infty,$$
 (33)

and

$$a_r < \infty$$
 if and only if $\int_0^1 \frac{D(s)}{s} ds < \infty$. (34)

When free boundaries exist, we can easily find them from the solution in the flux-saturation plane (cf. Figure 3). Using (27) we obtain

$$a_l = 2\frac{dy}{df}(1),$$

and similarly,

$$a_r = 2\frac{dy}{df}(0).$$

The behaviour of the solution in the neighbourhood of the free boundary follows directly from the differential equations (20) and (21). We have

$$\frac{1}{2}a_l = \lim_{\eta \downarrow a_l} \frac{(D(f)f')'(\eta)}{-f'(\eta)} h_l = \lim_{\eta \downarrow a_l} \frac{D(f(\eta))}{1 - f(\eta)} f'(\eta) h_l, \tag{35}$$

$$-\frac{1}{2}a_r = \lim_{\eta \uparrow a_r} \frac{\left(D(f(\eta))f'(\eta)\right)'}{f'(\eta)} h_r = \lim_{\eta \uparrow a_r} \frac{D(f(\eta))}{f(\eta)} f'(\eta) h_r. \tag{36}$$

These expressions imply that

$$\lim_{\eta \downarrow a_{l}} f'(\eta) \begin{cases} = 0 & \text{if } D'(1^{-}) = -\infty, \\ \in (-\infty, 0) & \text{if } D'(1^{-}) \in (-\infty, 0), \\ = -\infty & \text{if } D'(1^{-}) = 0, \end{cases}$$
(37)

and

$$\lim_{\eta \uparrow a_r} f'(\eta) \begin{cases} = 0 & \text{if } D'(0^+) = \infty, \\ \in (-\infty, 0) & \text{if } D'(0^+) \in (0, \infty), \\ = -\infty & \text{if } D'(0^+) = 0. \end{cases}$$
(38)

Expressions (35) and (36) can also be obtained by relating the speed of the free boundaries in the x, t-plane to the speed of the fluid particles. For instance,

$$\dot{x}_r(t) = \frac{a_r}{2\sqrt{t}} = \lim_{x \uparrow x_r(t)} \frac{\text{flux}(x,t)}{\phi_r u(x,t)}$$

$$= \lim_{x \uparrow x_r(t)} \frac{-h_r D(u) \partial u / \partial x(x,t)}{u(x,t)}$$

$$= -\frac{h_r}{\sqrt{t}} \lim_{\eta \uparrow a_r} \frac{D(f(\eta)) f'(\eta)}{f(\eta)}.$$

Finally we observe that volume (or mass) conservation is ensured by the continuity of the flux. Mathematically this is expressed by

$$\phi_l \int_{a_l}^0 (1 - f(\eta)) d\eta = \phi_r \int_0^{a_r} f(\eta) d\eta,$$

indicating that the volume of the oil penetrating the water is equal to the volume of water penetrating the oil.

4 Examples: Brooks-Corey and Van Genuchten models

In this section we consider two examples of capillary diffusion, each for different capillary-hydraulic properties of the porous medium. The Leverett *J*-function reflects the capillary properties of the porous medium, the relative permeabilities reflect its hydraulic properties. We shall consider here two different sets of functions which are frequently used in hydrology: the Brooks-Corey functions and the Van Genuchten functions.

For a Brooks-Corey medium, the Leverett J-function is given by

$$J(u) = u^{-1/\lambda}$$

with $\lambda > 0$, and the relative permeabilities are given by

$$k_{rw}(u) = u^{3+2/\lambda}, \qquad k_{rn}(u) = (1-u)^2(1-u^{1+2/\lambda}).$$

For a Van Genuchten medium J is given by

$$J(u) = (u^{-1/m} - 1)^{1-m},$$

with 0 < m < 1, and the relative permeabilities are given by

$$k_{rw}(u) = u^{1/2} \left(1 - (1 - u^{1/m})^m \right)^2, \qquad k_{rn}(u) = (1 - u)^{1/2} (1 - u^{1/m})^{2m}.$$

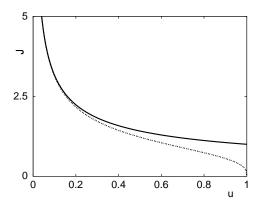


Figure 5: A Brooks-Corey J-curve for $\lambda = 2$ (solid), and a Van Genuchten J-curve for m = 2/3 (dashed).

The parameters λ and m are related to the distribution of the pore sizes in the porous medium. In Figure 5 we have given the graphs of a Brooks-Corey and a Van Genuchten J-curve. The parameters λ and m were chosen such that both curves have the same asymptotic behaviour as the saturation u tends to zero.

The important difference between the two cases is that Brooks-Corey has a nonzero entry pressure, whereas Van Genuchten has J(1) = 0. Consequently, the second (pressure) interface condition for a Van Genuchten medium is continuity of the capillary pressure, while for a Brooks-Corey medium the second interface condition is given by the extended pressure condition.

The extended pressure condition for a Brooks-Corey curve leads to the following relation between u_l and u_r when $h_l > h_r$:

$$u_r = \begin{cases} u_l/u^* & \text{if } 0 \le u_l \le u^*, \\ 1 & \text{if } u^* \le u_l \le 1, \end{cases}$$
 (39)

with

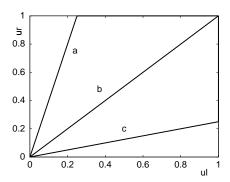
$$u^* = \left(\frac{h_r}{h_l}\right)^{\lambda}. (40)$$

To obtain the interface condition if $h_l < h_r$, we have to interchange u_l and u_r as well as h_l and h_r in (39) and (40).

The interface condition for a Van Genuchten type of medium is given by

$$u_r = \begin{cases} \left(1 + (h_r/h_l)^{1/(1-m)} \left(u_l^{-1/m} - 1\right)\right)^{-m} & \text{if } 0 < u_l \le 1, \\ 0 & \text{if } u_l = 0. \end{cases}$$

The graphs of the relations between u_r and u_l for the Brooks-Corey and the Van Genuchten model are given in Figure 6.



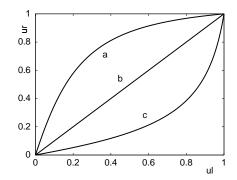


Figure 6: Second interface condition for a Brooks-Corey (left) and a Van Genuchten (right) medium, with $\lambda = 2$ and m = 2/3, for different ratios of h_r/h_l : (a) 0.5, (b) 1, (c) 2.

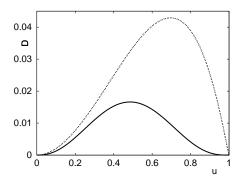


Figure 7: Diffusion functions of a Brooks-Corey (solid) and a Van Genuchten (dashed) medium, for $\lambda = 2$, m = 2/3 and $N_c = M = 1$.

The graphs of the diffusion functions for each type of medium are given in Figure 7. Note that in both cases D(0) = D(1) = 0. Hence free boundaries may occur.

The diffusion function (12) for a Brooks-Corey medium has the asymptotic behaviour:

$$D(u) \sim \frac{1}{\lambda} u^{2+1/\lambda}$$
 as $u \downarrow 0$, (41)

$$D(u) \sim \frac{2+\lambda}{\lambda^2} (1-u)^3 \quad \text{as } u \uparrow 1.$$
 (42)

Therefore, the integrability conditions in (33) and (34) are satisfied for all $\lambda > 0$. Hence we have free boundaries as $u \uparrow 1$ and as $u \downarrow 0$ for all $\lambda > 0$. Furthermore we see from (41) and (42) that $D'(0^+) = 0$ and $D'(1^-) = 0$ for all $\lambda > 0$. Therefore, the similarity solution satisfies $f'(a_r^-) = -\infty$ and $f'(a_l^+) = -\infty$ for all $\lambda > 0$.

Value	Parameter	Value
1	M	1
1	k_r	0.3
1	ϕ_r	1
2	m	2/3
	1 1 1 2	$ \begin{array}{cccc} 1 & M \\ 1 & k_r \\ 1 & \phi_r \end{array} $

Table 1: Data set of parameters

The diffusion function for a Van Genuchten medium yields:

$$D(u) \sim m(1-m)u^{(2+m)/2m} \text{ as } u \downarrow 0, \tag{43}$$

$$D(u) \sim \frac{1-m}{m^{m+1}} (1-u)^{m+1/2} \text{ as } u \uparrow 1.$$
 (44)

Again the integrability conditions in (33) and (34) are satisfied, now for all relevant values values of m (0 < m < 1). Further, we obtain from (43) that $D'(0^+) = 0$ for all 0 < m < 1, and from (44) that

$$D'(1^{-}) = \begin{cases} -\infty & \text{if } 0 < m < \frac{1}{2}, \\ -\sqrt{2} & \text{if } m = \frac{1}{2}, \\ 0 & \text{if } \frac{1}{2} < m < 1. \end{cases}$$
 (45)

So, the similarity solution satisfies $f'(a_r^-) = -\infty$ for all 0 < m < 1, and

$$f'(a_l^+) = \begin{cases} 0 & \text{if } 0 < m < \frac{1}{2}, \\ a_l/(2h_l\sqrt{2}) & \text{if } m = \frac{1}{2}, \\ -\infty & \text{if } \frac{1}{2} < m < 1. \end{cases}$$

In Figures 8 and 9, solutions corresponding to a Brooks-Corey and a Van Genuchten medium are shown as curves in the flux-saturation plane and as similarity profiles $f = f(\eta)$. The data are given in Table 1.

Note that for this data set the capillary pressure for the solution corresponding to the Brooks-Corey medium is discontinuous at the origin $(f_l > u^*)$. Further note that the nonwetting front $(\eta = a_l)$ for the solution corresponding to the Van Genuchten medium is much further to the left than the nonwetting front for the solution corresponding to the Brooks-Corey medium. This is due to the diffusion near f = 1 which is much greater for a Van Genuchten medium than for a Brooks-Corey medium because of the steeper slope of the J-curve near f = 1 (cf. Figure 5 and 7). Therefore, in a Van Genuchten medium the nonwetting phase easier enters the region originally occupied by the wetting phase than in a Brooks-Corey medium.

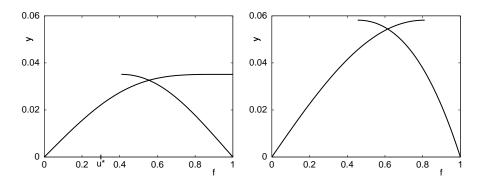


Figure 8: Solutions in the flux-saturation plane for a Brooks-Corey (left) and a Van Genuchten type of porous medium (right).

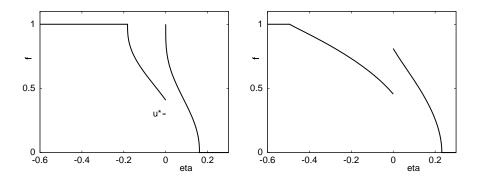


Figure 9: Similarity profiles $f = f(\eta)$ for a Brooks-Corey (left) and a Van Genuchten (right) porous medium.

For both types of porous media we can say more about the way the solution approaches the free boundaries. Substituting the asymptotic formulas (41) and (42) into (35) and (36), we obtain for a Brooks-Corey medium

$$\frac{h_l(2+\lambda)}{\lambda^2}(1-f(\eta))^2 f'(\eta) \to \frac{1}{2}a_l \quad \text{as } \eta \downarrow a_l,$$

and therefore

$$1 - f \sim K_1^{bc} (\eta - a_l)^{1/3}$$
 as $\eta \downarrow a_l$

with

$$K_1^{bc} = \left(\frac{3|a_l|\lambda^2}{2(2+\lambda)h_l}\right)^{1/3}.$$

Similarly, as f tends to zero we find

$$f \sim K_0^{bc} (a_r - \eta)^{\lambda/(1+2\lambda)}$$

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with

$$K_0^{bc} = \left(\frac{a_r(1+2\lambda)}{2h_r}\right)^{\lambda/(1+2\lambda)}.$$

In the case of a Van Genuchten medium we find

$$1 - f \sim K_1^{vg} (\eta - a_l)^{2/(2m+1)}$$
 as $\eta \downarrow a_l$,
 $f \sim K_0^{vg} (a_r - \eta)^{2m/(m+2)}$ as $\eta \uparrow a_r$,

with

$$K_1^{vg} = \left(\frac{|a_l|(2m+1)m^{m+1}}{4h_l(1-m)}\right)^{2/(2m+1)}$$
 and $K_0^{vg} = \left(\frac{a_r(m+2)}{4h_rm^2(1-m)}\right)^{2m/(m+2)}$.

Finally we show in Figure 10 the time-dependent behaviour of the Brooks-Corey similarity solution. Observe that the values at the origin are fixed and that the behaviour near the free boundaries remains unchanged, except for the \sqrt{t} scaling in the coefficients K_1^{bc} and K_0^{bc} . Furthermore we note that for fixed x < 0, $\lim_{t\to\infty} u(x,t) = f_l \in (0,1)$, while for fixed x > 0 $\lim_{t\to\infty} u(x,t) = f_r = 1$.

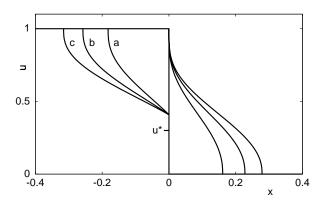


Figure 10: Similarity solution in a Brooks-Corey medium for (a) t = 1, (b) t = 2 and (c) t = 3, and the initial distribution.

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