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Semianalytical Solution for Two-Phase Flow in Porous Media with a Discontinuity

Radek Fučík, Jiří Mikyška, Michal Beneš,* and Tissa H. Illangasekare

We present a benchmark solution for one-dimensional porous media with heterogeneity involving two soils separated by a sharp interface. A similar problem was discussed previously by other researchers; however, only a diffusion term was considered in their models. The proposed solution allows the inclusion of advection terms in a limited way. This solution is useful in the verification of more complex numerical models of multiphase flow developed for general applications involving heterogeneous aquifers. A derivation of the semianalytical solution for heterogeneous porous media is presented and its existence and uniqueness are discussed. A computationally efficient algorithm and several computational results are presented.

Advanced numerical codes for multiphase flow through heterogeneous porous media such as those described by Helmig (1997), Mikyška et al. (2004), and Mikyška and Illangasekare (2005) require verification to assure that the governing equations are solved correctly before applying them to practical simulations. Code verification using the closed-form analytical solutions to the governing equations allows estimation of the accuracy of numerical schemes. Two well-known one-dimensional solutions of the two-phase flow problem in a homogeneous porous medium are the Buckley–Leverett solution for flow without capillary effects (e.g., Helmig, 1997, p. 177; LeVeque, 2002) and the semianalytical solution derived by McWhorter and Sunada (1990), with subsequent discussions by Chen et al. (1992), McWhorter and Sunada (1992), and Fučík et al. (2005, 2007). The semianalytical solution by McWhorter and Sunada (1992) includes both advective and capillary effects. We present the extension of this type of solution for the case of a heterogeneous porous medium with a simple discontinuity.

Since most natural systems are heterogeneous, numerical codes need to be verified on problems involving heterogeneous media. This is possible in a case of a simple heterogeneity. Such exact solutions exist for the diffusion case only (Philip, 1991; Raats and van Duijn, 1995; van Duijn and de Neef, 1998; Philip and van Duijn, 1999; Heinen and Raats, 1999) or for the stationary advection–diffusion case (Yortsos and Chang, 1990). Currently, however, there are no closed-form solutions available for this task when advection, diffusion, and accumulation terms are all included in the equation. In our case, we coupled the analytical solutions for flow in both homogeneous subdomains by a specific type of interfacial condition. The solution of the flow through a heterogeneous medium is then obtained by iteration. The form of proposed model does not, however, allow simulation of the trapping effect discussed by Helmig (1997, p. 264) and experimentally observed by Illangasekare et al. (1995).

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Formulation of the Flow Problem in a Homogeneous Medium

A one-dimensional problem describing flow of two incompressible immiscible liquids through a porous medium was considered where the wetting phase (water, indexed by w) displaces the nonwetting fluid (air or oil, indexed by n) in the horizontal direction (without the influence of gravity).

Let S be the effective wetting-phase saturation defined by $S = (S_w - S_{wr})/(1 - S_{wr} - S_{nr})$, where S_w is the wetting-phase saturation and S_{wr} and S_{nr} are the residual saturation of the wetting and nonwetting phase, respectively (Helmig, 1997, p. 54).

The governing equation for the unknown effective wetting-phase saturation function $S = S(t,x)$, where t is time and x is the spatial coordinate, has the form

$$\Phi\vartheta\frac{\partial S}{\partial t}=-q_t\frac{\partial f(S)}{\partial x}+\frac{\partial}{\partial x}\left[D(S)\frac{\partial S}{\partial x}\right] \quad [1]$$

where Φ is the porosity, q_t is the total flux, and ϑ stands for $(1 - S_{wr} - S_{nr})$. The capillary-hydraulic properties of the fluid–porous medium system are reflected in the functions f and D, where $f = f(S)$ is the fractional flow function and $D = D(S)$ is the diffusion coefficient that includes the capillary effects (see Fučík et al., 2007).

In our approach to flow through the heterogeneous medium, we relied on the fact that Eq. [1] can be treated analytically in each homogeneous subdomain provided that the following settings are considered. The initial condition and boundary conditions at $x = 0$ and $x \to +\infty$ are in the form

$$S(t,0)=S_0 \quad [2]$$

$$S(t,+\infty)=S_i \quad [3]$$

$$S(0,x)=S_i \quad [4]$$

for all $x \in (0,+\infty)$ and $t \in [0,+\infty)$. The flux of the displacing wetting phase (q_w) at $x = 0$ is given by

$$q_w(t,0)=q_0(t):=At^{-1/2} \quad [5]$$

where A depends on S_0 and S_i (McWhorter and Sunada, 1990). The value of A will follow from the derivation of the semianalytical solution. The other-phase velocities at $x = 0$ and at $x \to +\infty$ are unknown, although one can suppose that the boundary at $x \to +\infty$ is semipermeable, characterized by a constant scalar coefficient R. Assuming time-dependent input flux $q_w(t,0) = q_0(t)$ at $x = 0$, the total flux $q_t = q_w + q_n$ is constant in space and given as $q_t(t) = Rq_0(t)$ (McWhorter and Sunada, 1990).

The displaced nonwetting phase leaves the domain at $x \to +\infty$ or $x = 0$ depending on the parameter R. Since $q_t = q_w + q_n$, the nonwetting phase flux at $x = 0$ is given in the form

$$q_n(t,0)=A(R-1)t^{-1/2} \quad [6]$$

Originally, McWhorter and Sunada (1990) considered $R \in \{0,1\}$ only, indicating that either the unidirectional ($R = 1$) or the bidirectional ($R = 0$) displacement occurs. In the first case, the unidirectional displacement implies that the total flux is equal to the flux of the displacing phase at $x = 0$; that is, $q_t(t) = q_0(t)$ for all $t > 0$ and the nonwetting phase is being drained at $x \to +\infty$. In case of the bidirectional displacement, the outflow of the nonwetting phase is prevented at $x \to +\infty$. This means that the total flux equals zero, i.e., $q_t(t) = 0$ for all $t > 0$. Therefore, the phases have opposite fluxes for all $x \in [0,+\infty)$.

The formulation of the McWhorter and Sunada problem can be further generalized by allowing the parameter $R \in [0,1]$ (see Fučík et al., 2007). In this work, we further allow $R \in (-\infty,1]$. If we assume that the displaced phase is injected instead of being drained out at $x \to +\infty$, then a negative value of R can be prescribed. The displacing phase thus flows in the countercurrent flow direction of the total flux q_t. This generalization is important because it allows extension of the semianalytical solutions to a porous medium with a discontinuity.

Solution of the Flow Problem in Homogeneous Subdomains

Assume first that the boundary saturation S_0 is greater than the initial saturation S_i. This means that the wetting phase enters the semi-infinite domain $(0,+\infty)$ at $x = 0$, so that the parameter A is strictly positive. The other case, $S_0 < S_i$, where $A < 0$, will be discussed separately below.

The function F is introduced as

$$F=\varphi-\frac{D}{At^{-1/2}\left[1-Rf(S_i)\right]}\frac{\partial S}{\partial x} \quad [7]$$

where φ is given by

$$\varphi=R\frac{f-f(S_i)}{1-Rf(S_i)} \quad [8]$$

A substitution

$$\lambda\left[S(t,x)\right]=xt^{-1/2} \quad [9]$$

where the relationship $\lambda = \lambda(S)$ is assumed to be monotonous (see Fučík et al., 2007) reveals that $F = F(S)$. The substitution of Eq. [9] into the two-phase flow Eq. [1] is described in Appendix A. Consequently, the solution of Eq. [1] is obtained in the inverted form

$$\frac{2A\left[1-Rf(S_i)\right]}{\Phi\vartheta}\frac{dF}{dS}\left[S(t,x)\right]=xt^{-1/2} \quad [10]$$

for all values of $S \in [S_i,S_0]$. The function F is obtained from the integral equation

$$F(S)=1-\frac{\displaystyle\int_S^{S_0}\frac{(v-S)D(v)}{F(v)-\varphi(v)}dv}{\displaystyle\int_{S_i}^{S_0}\frac{(v-S_i)D(v)}{F(v)-\varphi(v)}dv} \quad [11]$$

and the value of A (related to S_0, S_i, and R) is given by

$$A^2=\frac{1}{2\left[1-Rf_w(S_i)\right]^2}\int_{S_i}^{S_0}\frac{(v-S_i)D(v)}{F(v)-\varphi(v)}dv \quad [12]$$

For given values of S_0, S_i, and R, the integral Eq. [11] has first to be solved to obtain function $F(S)$. This is done using iterative methods described in the Appendix B. Once the function $F(S)$ is known, the value of A is determined from Eq. [12]. Finally, as both $F(S)$ and A are known, the value of $S(t,x)$ can be determined from Eq. [10] in the inverse form, i.e., for given values of S and t, the position x is computed from Eq. [10] such that $S = S(t,x)$ holds. In this way, the semianalytical solution can be constructed.

In the case of $S_0 < S_i$, we use the following substitutions:

$$S_n = 1 - S \quad [13]$$

$$f_n(S_n) = f(1 - S_n) \quad [14]$$

$$D_n(S_n) = D(1 - S_n) \quad [15]$$

$$A_n = A(R - 1) \quad [16]$$

$$R_n = \frac{R}{R-1} \quad [17]$$

to transform Eq. [1] into

$$\Phi\vartheta \frac{\partial S_n}{\partial t} = -q_t \frac{\partial f_n(S_n)}{\partial x} + \frac{\partial}{\partial x}\left[D_n(S_n)\frac{\partial S_n}{\partial x}\right] \quad [18]$$

Equation [18] is formally the same as Eq. [1], with the initial and boundary conditions such that $S_{n0} > S_{ni}$. The substitutions of Eq. [16] and [17] allow the fluxes to be expressed in the form of $q_n = A_n t^{-1/2}$ and $q_t = R_n A_n t^{-1/2}$, respectively. Therefore, the semianalytical solution can be obtained as in the case of Eq. [1]. It follows from Eq. [16] that the value of A is negative in this case since the wetting phase flows out at $x = 0$, $A_n > 0$, and $R_n \in (-\infty,1)$. Negative values of A do not affect the formal derivation of the solution due to the square of A in Eq. [12].

The modified iteration method of Eq. [50] in Appendix B is efficient for values of $R \in [0,1]$; however, it does not seem to converge if a negative value of R is prescribed. On the other hand, the original method of McWhorter and Sunada (1990; Eq. [48] in Appendix B) works for $R < 0$. Therefore, we suggest obtaining the semianalytical solution using either the original iteration method (Eq. [48]) for negative values of R or the modified iteration method (Eq. [50]) for positive values of R.

Flow Problem in a Heterogeneous Porous Medium

We extend the ideas of van Duijn and de Neef (1998), who presented similarity solutions for two-phase flow in heterogeneous porous media for capillary redistribution problems without gravity:

$$\Phi\vartheta \frac{\partial S}{\partial t} = \frac{\partial}{\partial x}\left[D(S)\frac{\partial S}{\partial x}\right] \quad [19]$$

Equation [19] is obtained from Eq. [1] when $q_t = 0$.

Consider two semi-infinite one-dimensional porous media domains $(-\infty,0)$ and $(0,+\infty)$ of different material properties with an interface at $x = 0$. At $t = 0$, both domains contain the wetting phase with initial saturations S_i^r and S_i^l, where the superscripts l and r denote the two domains. The initial state is illustrated in Fig. 1. Both wetting and nonwetting fluxes are continuous across the material interface, i.e.,

$$q_\alpha^l(t,0) = q_\alpha^r(t,0), \quad \text{for all } t \geq 0, \quad \alpha \in \{w,n\} \quad [20]$$

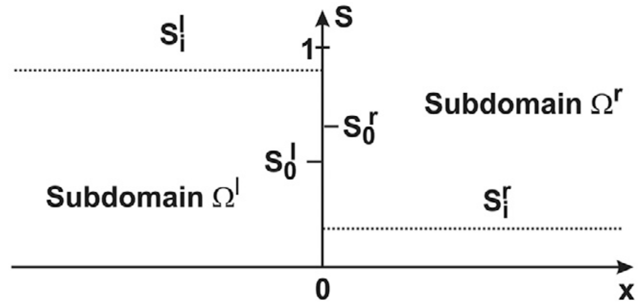

FIG. 1. Initial state of the porous medium with a soil texture discontinuity.

According to van Duijn et al. (1995), the saturation jump at the interface is modeled by the extended capillary pressure condition, formulated as

$$S^B = \begin{cases} 1 & \text{if } p_c^A\left(S^A\right) \leq p_c^B(1) \\ \left(p_c^B\right)^{-1}\left[p_c^A\left(S^A\right)\right] & \text{else} \end{cases} \quad [21]$$

where $(A,B) = (l,r)$ or $(A,B) = (r,l)$ is chosen in such a way that B denotes the subdomain with higher entry pressure. Nontrivial semianalytical solutions at the subdomains can be obtained only if $q_n \neq 0$. Therefore, we do not handle the trapping effects by this solution and we have to assume that the capillary pressure is continuous across the interface.

Van Duijn and de Neef (1998) derived the similarity solution as a combination of two solutions in semi-infinite domains by implementing the interface conditions of Eq. [20] and the continuity of capillary pressures of Eq. [21]. We apply their idea to Eq. [1] in both subdomains, Ω^l and Ω^r, including the advection term.

Coupling of Problems

We denote the indices characterizing the material in Ω^r and Ω^l by the superscripts r and l, respectively. Under this notation, the system of the two-phase flow equations can be given as

$$\Phi^r\vartheta^r \frac{\partial S}{\partial t} = -q_t \frac{\partial f^r(S)}{\partial x} + \frac{\partial}{\partial x}\left[D^r(S)\frac{\partial S}{\partial x}\right] \quad \text{in } \Omega^r \quad [22]$$

$$\Phi^l\vartheta^l \frac{\partial S}{\partial t} = -q_t \frac{\partial f^l(S)}{\partial x} + \frac{\partial}{\partial x}\left[D^l(S)\frac{\partial S}{\partial x}\right] \quad \text{in } \Omega^l \quad [23]$$

The initial and boundary conditions described below are given such that the semianalytical solution can be obtained in both subdomains (see above).

For Ω^r, we set

$$S(t,0) = S_0^r \quad \text{for all } t > 0 \quad [24]$$

$$S(t,+\infty) = S_i^r \quad \text{for all } t > 0 \quad [25]$$

$$S(0,x) = S_i^r \quad \text{for all } x > 0 \quad [26]$$

while for Ω^l, we set

$$S(t,0)=S_0^{\mathrm{l}} \quad \text{for all } t>0 \tag{27}$$

$$S(t,-\infty)=S_{\mathrm{i}}^{\mathrm{l}} \quad \text{for all } t>0 \tag{28}$$

$$S(0,x)=S_{\mathrm{i}}^{\mathrm{l}} \quad \text{for all } x<0 \tag{29}$$

The wetting flux is given as $q_{\mathrm{w}}^{\mathrm{r}}(t,0) = A^{\mathrm{r}}t^{-1/2}$ for Ω^{r} and using the definition of the ratio R in Eq. [6], the total flux becomes $q_{\mathrm{t}}(t) = A^{\mathrm{r}}Rt^{-1/2}$. The unknown parameters S_0^{l} and S_0^{r} will be determined as a result of the continuity of the fluxes in Eq. [20] and the continuity of capillary pressures.

We transform the problem in Ω^{l} to take advantage of the McWhorter and Sunada (1990) semianalytical solution. This is done by a substitution of $\tilde{x} = -x$ in Ω^{l}. The transformed wetting-phase flux $\tilde{q}_{\mathrm{w}}^{\mathrm{l}}$ at $\tilde{x} = 0$ becomes

$$\tilde{q}_{\mathrm{w}}^{\mathrm{l}}(t,0)=A^{\mathrm{l}}t^{-1/2} \tag{30}$$

At the interface, the wetting-phase flux is continuous Eq. [20], which allows coupling of both left and right subdomain problems together by the following (fluxes have opposite signs after the transformation $\tilde{x} = -x$):

$$A^{\mathrm{l}}=-A^{\mathrm{r}} \tag{31}$$

The total flux is constant in space throughout both subdomains and continuous across the interface. The value of the transformed total flux is $\tilde{q}_{\mathrm{t}} = -q_{\mathrm{t}} = -A^{\mathrm{r}}Rt^{-1/2} = A^{\mathrm{l}}Rt^{-1/2}$. Consequently, the same value of the parameter R must be used in both subdomains.

The negative value of the flux in the McWhorter and Sunada (1990) formulation corresponds to the fact that $S_0 < S_{\mathrm{i}}$. Thus, to obtain a positive value of A in one subdomain and a negative value of A in the other subdomain (c.f., Eq. [31]), either

$$S_0^{\mathrm{l}}>S_{\mathrm{i}}^{\mathrm{l}} \quad \text{and} \quad S_0^{\mathrm{r}}<S_{\mathrm{i}}^{\mathrm{r}} \tag{32}$$

or

$$S_0^{\mathrm{l}}<S_{\mathrm{i}}^{\mathrm{l}} \quad \text{and} \quad S_0^{\mathrm{r}}>S_{\mathrm{i}}^{\mathrm{r}} \tag{33}$$

must hold.

The continuity of capillary pressures provides the common value of interfacial capillary pressure (p_{c}^0) in the form

$$p_{\mathrm{c}}^0 := p_{\mathrm{c}}^{\mathrm{r}}\left(S_0^{\mathrm{r}}\right)= p_{\mathrm{c}}^{\mathrm{l}}\left(S_0^{\mathrm{l}}\right) \tag{34}$$

As the capillary pressure is a strictly decreasing function of water saturation, Eq. [32] and [33] together with Eq. [34] imply that

$$p_{\mathrm{c}}^{\mathrm{r}}\left(S_{\mathrm{i}}^{\mathrm{r}}\right)< p_{\mathrm{c}}^0 < p_{\mathrm{c}}^{\mathrm{l}}\left(S_{\mathrm{i}}^{\mathrm{l}}\right) \tag{35}$$

or

$$p_{\mathrm{c}}^{\mathrm{l}}\left(S_{\mathrm{i}}^{\mathrm{l}}\right)< p_{\mathrm{c}}^0 < p_{\mathrm{c}}^{\mathrm{r}}\left(S_{\mathrm{i}}^{\mathrm{r}}\right) \tag{36}$$

respectively. Taking into account that p_{c}^0 must be greater than $p_{\mathrm{c}}^{\max}$, where

$$p_{\mathrm{c}}^{\max} := \max\left\{p_{\mathrm{c}}^{\mathrm{l}}(1), p_{\mathrm{c}}^{\mathrm{r}}(1)\right\} \tag{37}$$

(otherwise the capillary pressure prevents flow of the nonwetting phase across the interface and continuity of the capillary pressure cannot be established), we finally obtain a range for $p_{\mathrm{c}}^0 \in (p_{\min}, p_{\max})$, where

$$p_{\max} := \max\left\{p_{\mathrm{c}}^{\mathrm{l}}\left(S_{\mathrm{i}}^{\mathrm{l}}\right), p_{\mathrm{c}}^{\mathrm{r}}\left(S_{\mathrm{i}}^{\mathrm{r}}\right)\right\} \tag{38}$$

and

$$p_{\min} := \max\left\{p_{\mathrm{c}}^{\max}, \min\left[p_{\mathrm{c}}^{\mathrm{l}}\left(S_{\mathrm{i}}^{\mathrm{l}}\right), p_{\mathrm{c}}^{\mathrm{r}}\left(S_{\mathrm{i}}^{\mathrm{r}}\right)\right]\right\} \tag{39}$$

The existence of the semianalytical solution of the McWhorter and Sunada (1990) problem for the porous medium with a discontinuity is equivalent to the existence of such saturations S_0^{l} and S_0^{r} that the condition Eq. [31] holds. Both A^{l} and A^{r} are functions of S_0^{l}, R, $S_{\mathrm{i}}^{\mathrm{l}}$, and S_0^{r}, R, $S_{\mathrm{i}}^{\mathrm{r}}$, respectively, but the explicit relationship fulfilling Eq. [31] is unknown. If the solution exists, then it is unique due to the monotonic relationship between A and S_0 (see Fučík et al., 2007).

Computational Algorithm

Let $S_{\mathrm{i}}^{\mathrm{l}}$, $S_{\mathrm{i}}^{\mathrm{r}}$, and R be given. The proposed algorithm is based on determining $p_{\mathrm{c}}^0 \in (p_{\min}, p_{\max})$, where the values $p_{\min}$ and $p_{\max}$ are given by Eq. [38] and [39], respectively. The boundary saturations S_0^{l} and S_0^{r} are computed knowing p_{c}^0 using the continuity of capillary pressures given by Eq. [34]. Consequently, the semianalytical solutions are obtained for each subdomain. As a result, the values of A^{l} and A^{r} are computed based on the values S_0^{l} and S_0^{r}, which are functions of p_{c}^0. Therefore A^{l} and A^{r} can be also be regarded as functions of p_{c}^0. The aim is to find a value of p_{c}^0 such that Eq. [31] holds, i.e., $A^{\mathrm{l}}(p_{\mathrm{c}}^0) + A^{\mathrm{r}}(p_{\mathrm{c}}^0) = 0$.

Denoting $\kappa(p_{\mathrm{c}}) = A^{\mathrm{l}}(p_{\mathrm{c}}) + A^{\mathrm{r}}(p_{\mathrm{c}})$, the value of p_{c}^0 is determined by the equation

$$\kappa\left(p_{\mathrm{c}}^0\right)=0 \tag{40}$$

We observe that $p_{\mathrm{c}}(S)$ is strictly decreasing (so is its inverse), and that $A^{\mathrm{l}} = A^{\mathrm{l}}(S^{\mathrm{l}})$, $A^{\mathrm{r}} = A^{\mathrm{r}}(S^{\mathrm{r}})$ are strictly increasing functions. This implies that $\kappa(p_{\mathrm{c}})$ is a monotonic function. The solution of Eq. [40] therefore can be found iteratively using the bisection method. Moreover, monotonicity of κ allows verification of the existence of the solution p_{c}^0 of Eq. [40] by considering the sign of $\kappa(p_{\min})$ and $\kappa(p_{\max})$ (see Step 2 below).

The bisection algorithm given below requires values of the function κ for several p_{c}^0. For a given p_{c}^0, the function $\kappa(p_{\mathrm{c}}^0)$ is evaluated as follows:

1. Boundary saturations S_0^{l} and S_0^{r} are obtained from p_{c}^0 using Eq. [34].
2. The semianalytical solutions in Ω^{l} and Ω^{r} are computed as above together with values of $A^{\mathrm{l}}(p_{\mathrm{c}}^0)$ and $A^{\mathrm{r}}(p_{\mathrm{c}}^0)$.
3. Set $\kappa(p_{\mathrm{c}}^0) = A^{\mathrm{l}}(p_{\mathrm{c}}^0) + A^{\mathrm{r}}(p_{\mathrm{c}}^0)$.

The bisection algorithm works as follows:

1. Let R, S_i^l, S_i^r and a tolerance $\varepsilon > 0$ be given. Determine p_{min} and p_{max} from Eq. [38] and [39], set $\underline{p} = p_{min}$ and $\overline{p} = p_{max}$.
2. Compute $\kappa(p_{max})$ and $\kappa(p_{min})$. If $\kappa(p_{max})\kappa(p_{min}) > 0$, then the problem cannot be solved due to physically unrealistic initial conditions (fluxes on the two sides are in opposite directions) and the algorithm is terminated.
3. Set $p_c^0 = 1/2(\underline{p} + \overline{p})$.
4. Evaluate $\kappa(p_c^0)$. If $|\kappa(p_c^0)| < \varepsilon$, then terminate the algorithm with success.
5. If $\kappa(p_c^0)\kappa(\underline{p}) > 0$, then set $\underline{p} := p_c^0$; otherwise set $\overline{p} := p_c^0$.
6. Continue with Step 3.

Computational Studies

For computations, the sands with properties given in Table 1 were used. The Brooks and Corey model (see Brooks and Corey, 1964) for capillary pressure was combined with the Burdine model of relative permeability (see Helmig, 1997, p. 75). As the wetting phase, water ($\mu_w = 0.001$ kg m^{-1} s^{-1}) was used, interacting with the nonwetting phase (tetrachloroethene, $\mu_n = 0.0009$ kg m^{-1} s^{-1}). The two-phase flow in one-dimensional heterogeneous medium described by Eq. [22] and [23] with corresponding conditions set up above was then solved for several choices of the initial conditions and of the values of the parameter R. The existence of the solution of Eq. [40] cannot be always guaranteed, however, as shown in Fig. 2a, where $S_i^l = 1$, $S_i^r = 0$, and $R = 0.95$. On the other hand, Fig. 2b to 2d indicate situations where the solution of Eq. [40] was found. Solvability of Eq. [40] is related to the choice of R and reflects the physical limitations of the problem formulation. This is illustrated in Fig. 3. The values of p_c^0 are limited by the minimal achievable capillary pressure p_{min} given by Eq. [39]. In Fig. 4, saturation profiles obtained for three different choices of initial conditions and for four different choices of the parameter R are shown. More computational studies and interactive implementation of the presented algorithm can be found at http://mmg.fjfi.cvut.cz/~fucik/hetero (verified 28 May 2008).

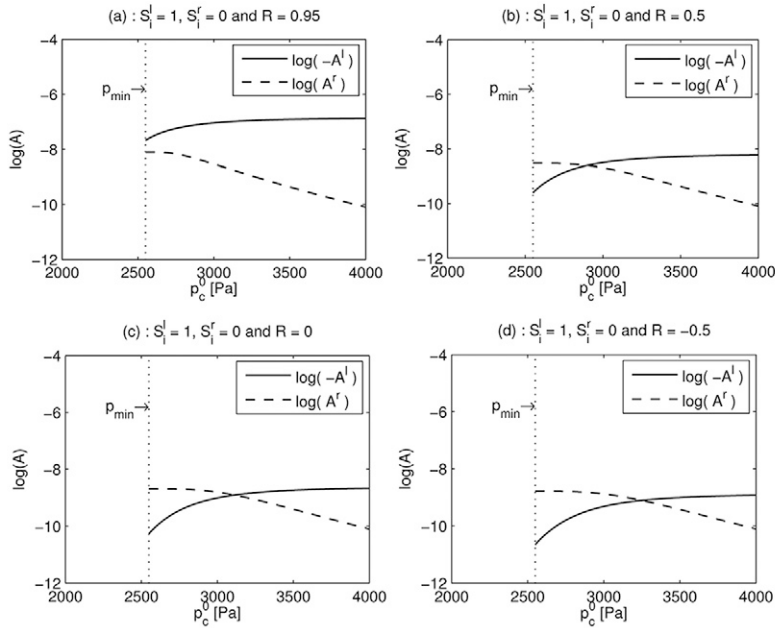

FIG. 2. Relationship between $-A^l$ and A^r (logarithmic scale is used) and p_c^0.

Conclusions

This study dealt with the semianalytical solution for two-phase flow in a simple heterogeneous medium consisting of two soils separated by a sharp interface. This result is based on the approach presented in McWhorter and Sunada (1990) and Fučík et al. (2007) dealing with the advection–diffusion problem in a homogeneous medium. Treatment of interfaces in a heterogeneous medium follows the formulation by Philip (1991), van Duijn and de Neef (1998), and Philip and van Duijn (1999), limited to the diffusion case only. Our approach allows consideration of diffusion together with advection, as there are many situations in two-phase flow where both advection and diffusion terms have to be considered. The solution is obtained by an iteration procedure working with the flow in both homogeneous subdomains to reach the required condition at the interface. The functionality of the algorithm is illustrated by means of several numerical examples using the Brooks and Corey model for the relative permeability and capillary pressure functions. Additionally, the conditions under which a solution exists are discussed as well.

TABLE 1. Parameter setup for coarse and fine sands according to de Neef and Molenaar (1997).

Parameter	Fine sand	Coarse sand
Porosity (Φ)	0.34	0.34
Intrinsic permeability (K), m^2	5.3×10^{-12}	7×10^{-12}
Residual water saturation (S_{wr})	0	0
Brooks–Corey entry pressure (P_d), Pa	2550	2218
Brooks–Corey pore size distribution index (λ)	2.48	2.48

Appendix A

Appendix A summarizes the steps leading to the analytical implicit formula solving Eq. [1]. It was derived by McWhorter and Sunada (1990) and further discussed in Fučík et al. (2007).

The transformation of Eq. [1] into Eq. [10] using the substitution of Eq. [9] is performed in the following steps. The substitution of Eq. [9] allows expression of the partial derivatives of $S(t,x)$ in the following form:

$$\frac{\partial S}{\partial x} = \left[\frac{d\lambda(S)}{dS}\right]^{-1} t^{-1/2} \quad \text{and} \qquad \frac{\partial S}{\partial t} = -\frac{1}{2}\left[\frac{d\lambda(S)}{dS}\right]^{-1} x t^{-3/2} \qquad [41]$$

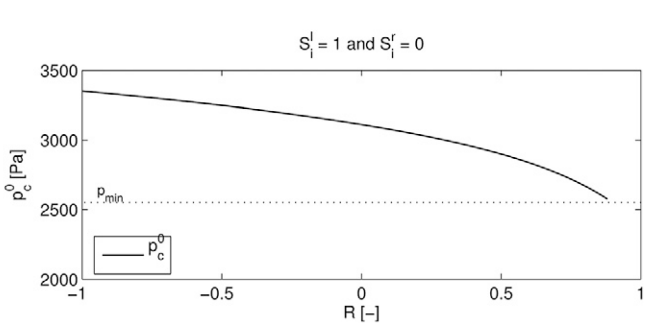

FIG. 3. Relationship between R and p_c^0.

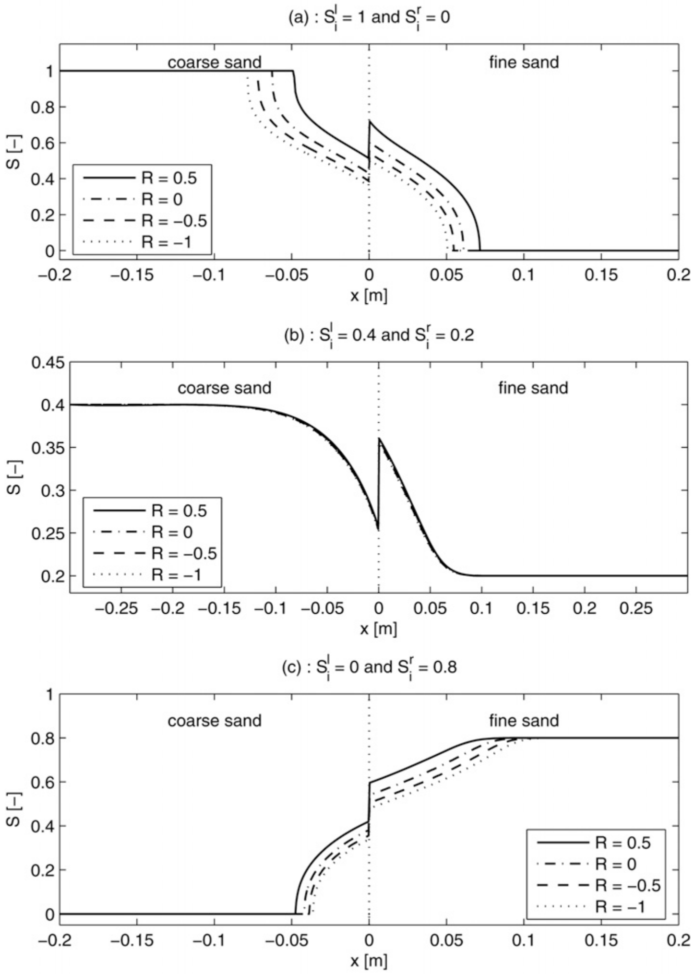

FIG. 4. Semianalytical solutions for a medium with a discontinuity for three different initial setups and various R at time t = 1000 s.

Substituting the partial derivative $\partial S/\partial x$ given by Eq. [41] into Eq. [7], we obtain

$$F = \varphi - \frac{D}{A\left[1 - Rf\left(S_\mathrm{i}\right)\right]}\left[\frac{\mathrm{d}\lambda(S)}{\mathrm{d}S}\right]^{-1} \qquad [42]$$

Consequently, F is expressed in terms of S only (variables x, t, and $\partial S/\partial x$ were eliminated), i.e., $F = F(S)$. Equation [7] allows us to rewrite Eq. [1] in terms of F as

$$\phi\vartheta\frac{\partial S}{\partial t} = -At^{-1/2}\left[1 - Rf\left(S_\mathrm{i}\right)\right]\frac{\partial F}{\partial x} \qquad [43]$$

Using the fact that $\partial F/\partial x = (\mathrm{d}F/\mathrm{d}S)(\partial S/\partial x)$, the substitution of Eq. [41] into Eq. [43] leads to

$$\begin{aligned}&-\Phi\vartheta\frac{1}{2}\left[\frac{\mathrm{d}\lambda(S)}{\mathrm{d}S}\right]^{-1} xt^{-3/2}\\ &= -At^{-1/2}\left[1 - Rf\left(S_\mathrm{i}\right)\right]\frac{\mathrm{d}F(S)}{\mathrm{d}S}\left[\frac{\mathrm{d}\lambda(S)}{\mathrm{d}S}\right]^{-1} t^{-1/2}\end{aligned} \qquad [44]$$

from which Eq. [10] follows directly.

To derive Eq. [11], Eq. [10] is differentiated with respect to S to obtain

$$\frac{\mathrm{d}^2F}{\mathrm{d}S^2}(S) = \frac{\Phi\vartheta}{2A\left[1 - Rf\left(S_\mathrm{i}\right)\right]}\frac{\mathrm{d}\lambda}{\mathrm{d}S} \qquad [45]$$

where we substitute for $\mathrm{d}\lambda/\mathrm{d}S$ from Eq. [42] to get the following differential equation for $F(S)$

$$\frac{\mathrm{d}^2F}{\mathrm{d}S^2}(S) = -\frac{\Phi\vartheta}{2A^2\left[1 - Rf\left(S_\mathrm{i}\right)\right]^2}\frac{D}{F(S) - \varphi(S)} \qquad [46]$$

This equation can be twice integrated. Using the conditions $F(S_0) = 1$ and $\mathrm{d}F/\mathrm{d}S = 0$, which follow from Eq. [2] and [3], respectively, we obtain

$$F(S) = 1 - \frac{\Phi\vartheta}{2A^2\left[1 - Rf\left(S_\mathrm{i}\right)\right]^2}\int_S^{S_0}\frac{(v - S)D(v)}{F(v) - \varphi(v)}\mathrm{d}v \qquad [47]$$

Taking into account that $F(S_\mathrm{i}) = 0$, Eq. [47] yields Eq. [12] for A. Finally, Eq. [47] can be rewritten by means of Eq. [12] into Eq. [11].

Appendix B

This appendix is devoted to the description of the iterative procedure for solving Eq. [11]. For given values of S_0, S_i, and R, the integral Eq. [11] has first to be solved to obtain the function $F(S)$. This is done iteratively and approximately, therefore the solution is referred to as semianalytical. McWhorter and Sunada (1992) suggested using $F_0(S) \equiv 1$ as a first iteration and evaluating the next iterations by substituting the previously obtained iteration of the function F into the right-hand side of the integral Eq. [11], i.e.,

$$F_{k+1}(S) = 1 - \frac{\displaystyle\int_S^{S_0}\frac{(v - S)D(v)}{F_k(v) - \varphi(v)}\mathrm{d}v}{\displaystyle\int_{S_\mathrm{i}}^{S_0}\frac{(v - S_\mathrm{i})D(v)}{F_k(v) - \varphi(v)}\mathrm{d}v} \qquad [48]$$

The iterations are terminated when $\|F_{k+1} - F_k\|_{L+\infty} < tol$, where tol is a user-defined tolerance. The iterative method of Eq. [48] does not converge for values of S_0 larger than a certain critical value S_0^{crit} if R is close to 1. This problem was analyzed in detail in Fučík et al. (2007), where an alternative iteration method was developed that works for all values of S_0 except for the case $R = 1$ and $S_0 \to 1$. In this method, the expression $G(S) = D(S)/[F(S) - \varphi(S)]$ is used to rewrite Eq. [11] as

$$F(S) = \frac{D(S)}{G(S)} + \varphi(S) = 1 - \frac{\displaystyle\int_S^{S_0}(v - S)G(v)\mathrm{d}v}{\displaystyle\int_{S_\mathrm{i}}^{S_0}(v - S_\mathrm{i})G(v)\,\mathrm{d}v} \qquad [49]$$

The iteration scheme for G has the following form

$$\begin{aligned}&G_{k+1}(S)\\ &= D(S) + G_k(S)\left[\varphi(S) + \frac{\displaystyle\int_S^{S_0}(v - S)G(v)\mathrm{d}v}{\displaystyle\int_{S_\mathrm{i}}^{S_0}(v - S_\mathrm{i})G(v)\,\mathrm{d}v}\right]\end{aligned} \qquad [50]$$

The initial guess $G_0(S) = D/(1 - \varphi)$ corresponds to the choice $F_0 \equiv 1$ in Eq. [48]. After each iteration, the value $F_{k+1}(S)$ can be computed from $G_{k+1}(S)$ as

$$F_{k+1}(S) = \frac{D(S)}{G_{k+1}(S)} + \varphi(S) \qquad [51]$$

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