

## EVALUATION OF SATURATION-DEPENDENT FLUX ON TWO-PHASE FLOW USING GENERALIZED SEMI-ANALYTIC SOLUTION

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**Abstract.** An important step in model development protocol is the verification of the model code. This is performed by comparing the code performance with existing analytical solutions under simplified conditions (e.g. geometry, flow dimensionality, parameter distribution and boundary conditions). Two closed form solutions are commonly used as benchmarks for the verification of two-phase flow in porous media codes: (1) Buckley-Leverett solution and (2) McWhorter and Sunada solution. The first assumes the capillary effects are negligible, and the second formulation includes capillary effects but assumes a particular functional form for the boundary flux that starts from a physically unrealistic infinity value. This paper presents a derivation that generalizes the boundary flux term by allowing it to start from a finite value. To expand the class of admissible boundary and initial conditions, we offer a numerical algorithm that solves the transport equation for phase saturations using the Finite-Difference Method in space and time. The use of the algorithm is demonstrated by conducting a series of computations in one-dimensional spatial domain. (see also our article in [2])

**Key words.** Multiphase flow code verification, McWhorter-Sunada's closed form solution, transport equation, Finite-Difference Method, heterogeneous media.

**AMS subject classifications.** 65M06, 65M20, 35K55, 76T99

**1. Model of multiphase flow.** McWhorter and Sunada [6] formulated the solution for a semi-infinite problem domain with specific boundary conditions to arrive at a close form analytical solution of the multiphase flow. For general setting see [4], for an application see [5]. The non-wetting phase (indexed  $n$ ) is displaced by the wetting liquid (water, indexed  $w$ ) horizontally with no gravity effect and assumed incompressibility of fluids.

This section contains the derivation of the multiphase flow equation. The Darcy law applied to the two fluid phases yields

$$q_w = -\frac{k_w}{\mu_w} \frac{\partial p_w}{\partial x}, \quad q_n = -\frac{k_n}{\mu_n} \frac{\partial p_n}{\partial x}, \quad (1.1)$$

where  $p_\alpha$  is the pressure,  $q_\alpha$  is the volumetric flux,  $k_\alpha$  is the hydraulic conductivity and  $\mu_\alpha$  is the dynamic viscosity for the phase denoted by  $\alpha$ . The total flux is denoted by  $q_t = q_w + q_n$  and the capillary pressure

$$p_c(S_w) = p_n - p_w. \quad (1.2)$$

The aim is to eliminate variables respective to the non-wetting phase i.e. the flux  $q_n$  and the pressure  $p_n$ . Subtraction of formulas in (1.1) yields

$$\frac{\partial p_n}{\partial x} - \frac{\partial p_w}{\partial x} = -q_n \frac{\mu_n}{k_n} + q_w \frac{\mu_w}{k_w}.$$

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Applying (1.2) and  $q_n = q_t - q_w$  we get

$$\begin{aligned} \frac{\partial p_c}{\partial x} &= -(q_t - q_w) \frac{\mu_n}{k_n} + q_w \frac{\mu_w}{k_w} = -q_t \frac{\mu_n}{k_n} + q_w \left( \frac{\mu_w}{k_w} + \frac{\mu_n}{k_n} \right), \\ \frac{k_n \frac{\mu_n}{k_n}}{\mu_n \frac{\mu_w}{k_w} + \frac{\mu_n}{k_n}} \frac{\partial p_c}{\partial x} &= -\frac{\mu_n}{\frac{\mu_w}{k_w} + \frac{\mu_n}{k_n}} q_t + q_w, \\ \underbrace{\frac{k_n}{\mu_n} \frac{1}{1 + \frac{k_n \mu_w}{k_w \mu_n}} \frac{d p_c}{d S_w}}_{-D(S_w)} \frac{\partial S_w}{\partial x} &= -\underbrace{\frac{1}{1 + \frac{k_n \mu_w}{k_w \mu_n}}}_{f(S_w)} q_t + q_w. \end{aligned}$$

Consequently

$$q_w = f(S_w) q_t - D(S_w) \frac{\partial S_w}{\partial x}, \quad (1.3)$$

with

$$f(S_w) = \frac{1}{1 + \frac{k_n(S_w) \mu_w}{k_w(S_w) \mu_n}}, \quad (1.4)$$

$$D(S_w) = -\frac{k_n(S_w) f(S_w)}{\mu_n} \frac{d p_c}{d S_w}(S_w). \quad (1.5)$$

Denoting  $\Phi$  as the porosity, the mass balance equation has the following form

$$\frac{\partial q_w}{\partial x} + \Phi \frac{\partial S_w}{\partial t} = 0. \quad (1.6)$$

Finally, using the expression (1.3) the *multiphase flow equation* is obtained as

$$\Phi \frac{\partial S_w}{\partial t} = -q_t \frac{d f}{d S_w} \frac{\partial S_w}{\partial x} + \frac{\partial}{\partial x} \left( D \frac{\partial S_w}{\partial x} \right). \quad (1.7)$$

We set the boundary and initial conditions as was proposed by McWhorter and Sunada [6]

$$\begin{aligned} q_w(t, 0) &= q_0(t) = A t^{-\frac{1}{2}}, \\ S_w(t, +\infty) &= S_i, \\ S_w(0, x) &= S_i, \end{aligned}$$

where  $A$  is the injection rate constant. Note that at  $t = 0$ , the boundary flux takes an unrealistic value of infinity.

**2. Analytical treatment.** As follows from [6], the *fractional flow function* is to be defined as

$$F(t, x) = \frac{\frac{q_w(t, x)}{q_0(t)} - f_i R}{1 - f_i R}, \quad \text{with} \quad R(t) = \frac{q_t(t)}{q_0(t)} \quad \text{and} \quad f_i = f(S_i). \quad (2.1)$$

For unidirectional displacement,  $q_t = q_0$  and  $F$  has the physical meaning of the ratio of net wetting phase flux at  $(x, t)$  to the net influx of wetting phase. In that case,  $R = 1$ . On the other hand,  $R = q_t = 0$  for counter-current flow, and again,  $F$  represents a flux ratio. (quoted the [6], p.401)

In fact, the indicator function  $R(t)$  is a constant independent on  $t$ . Regrouping the expression (2.1)

$$q_0(t)(1 - Rf_i)F(t, x) = q_w(t, x) - Rf_i q_0(t),$$

differentiating by  $\frac{\partial}{\partial x}$

$$q_0(t)(1 - Rf_i)\frac{\partial F}{\partial x}(t, x) = \frac{\partial q_w}{\partial x}(t, x),$$

and substituting into (1.6), the mass-balance equation becomes

$$At^{-\frac{1}{2}}(1 - Rf_i)\frac{\partial F}{\partial x}(t, x) + \Phi\frac{\partial S_w}{\partial t} = 0. \quad (2.2)$$

The following lines present the reduction of (2.2) into an ODE. Using the change of variables

$$(t, x, S_w, F) \longleftrightarrow (\tau, \lambda, \bar{S}_w, \bar{F}),$$

described by relations

$$\lambda = t^{-\frac{1}{2}}x, \quad S_w = \bar{S}_w, \quad t = \tau, \quad F = \bar{F},$$

with

$$S_w = S_w(t, x), \quad F = F(t, x), \quad \lambda = \lambda(\bar{S}_w), \quad \bar{F} = \bar{F}(\tau, \bar{S}_w),$$

the equation (2.2) is transformed into

$$\frac{2A(1 - Rf_i)}{\Phi}\frac{\partial \bar{F}}{\partial \bar{S}_w}(\tau, \bar{S}_w) = \lambda(\bar{S}_w). \quad (2.3)$$

The final form of the transformed fractional flow function  $\bar{F}$  is

$$\bar{F}(\bar{S}_w) = -\frac{\Phi}{2A^2(1 - Rf_i)^2}\int_{\bar{S}_w}^{S_0}\frac{(s - \bar{S}_w)D(s)}{\bar{F}(s) - f_n(s)}ds - \frac{d\bar{F}}{d\bar{S}_w}(S_0)(S_0 - \bar{S}_w) + \bar{F}(S_0), \quad (2.4)$$

where  $f_n$  is defined by

$$f_n = \frac{R(f - f_i)}{1 - Rf_i}.$$

The expression (2.4) is simplified by the condition

$$\frac{d\bar{F}}{d\bar{S}_w}(S_0) = 0,$$

which follows from (2.3) ( $S_0$  is achieved at  $x = 0$  for all  $t > 0$ ). It requires that

$$A^2 = \frac{\Phi}{2(1 - Rf_i)^2}\int_{S_i}^{S_0}\frac{(s - S_i)D(s)}{\bar{F}(s) - f_n(s)}ds. \quad (2.5)$$

Substituing (2.5) into (2.4) we get

$$\overline{F}(\overline{S}_w) = 1 - \frac{\int_{S_0}^{S_w} \frac{(s-\overline{S}_w)D(s)}{\overline{F}(s)-f_n(s)} ds}{\int_{S_i}^{S_0} \frac{(s-S_i)D(s)}{\overline{F}(s)-f_n(s)} ds}. \quad (2.6)$$

Together, (2.5) and (2.6) constitute an implicit expression for the dependence of  $S_0$  on  $A$ . Numerical computations proceed conveniently by prescribing  $S_0$ , calculating  $\overline{F}(\overline{S}_w)$  from (2.6) by iteration (see [6] for details), and finally, computing  $A$  from (2.5).

**Remark.** The numerical solution presented in Section 2 is compared to analytical solution obtained from [6]. Beside the error commented in [8] and replied in [7], it is essential to point out another error in the Appendix B of [6] concerning numerical realisation of the analytical solution. The equation ([6]:19) on page 402 is transformed into ([6]:B9) by substitution. The correct form of the ([6]:B9) is

$$\frac{dF}{dS} = \frac{1}{S_0 - S_i} \frac{\int_S^1 \frac{D_n(\beta)}{F(\beta)-f_n(\beta)} d\beta}{\int_0^1 \frac{\beta D_n(\beta)}{F(\beta)-f_n(\beta)} d\beta}.$$

**3. Suggestion to generalisation of the input flux.** Assuming  $q_0(t) = A g(t)$ , the equation (2.2) becomes

$$A g(t)(1 - Rf_i) \frac{\partial F}{\partial x}(t, x) + \Phi \frac{\partial S_w}{\partial t} = 0. \quad (3.1)$$

The change of variables  $(t, x, S_w, F) \longleftrightarrow (\tau, \lambda, \overline{S}_w, \overline{F})$  has the form

$$\lambda = x g(t), \quad S_w = \overline{S}_w, \quad t = \tau, \quad F = \overline{F},$$

with

$$S_w = S_w(t, x), \quad F = F(t, x), \quad \lambda = \lambda(\overline{S}_w), \quad \overline{F} = \overline{F}(\tau, \overline{S}_w).$$

To determine the form of  $g(t)$  it is necessary to follow these steps. Differentiating the expression

$$F(t, x) = \overline{F}(t, S_w(t, x)),$$

by  $\frac{\partial}{\partial x}$  we get

$$\frac{\partial F}{\partial x}(t, x) = \frac{\partial \overline{F}}{\partial \overline{S}_w}(t, S_w(t, x)) \frac{\partial S_w}{\partial x}(t, x).$$

Differentiating the expression

$$S_w \left( \tau, \frac{1}{g(\tau)} \lambda(\overline{S}_w) \right) = \overline{S}_w,$$

by  $\frac{\partial}{\partial \tau}$  we get

$$\frac{\partial S_w}{\partial t} \left( \tau, \frac{1}{g(\tau)} \lambda(\overline{S}_w) \right) - \frac{\dot{g}(\tau)}{g^2(\tau)} \lambda(\overline{S}_w) \frac{\partial S_w}{\partial x} \left( \tau, \frac{1}{g(\tau)} \lambda(\overline{S}_w) \right) = 0,$$

where  $\dot{g}(\tau)$  stands for  $\frac{d}{d\tau}g(\tau)$ . The equation (3.1), after substitution of the above expressions, becomes

$$Ag(\tau)(1 - Rf_i)\frac{\partial \bar{F}}{\partial \bar{S}_w}\frac{\partial S_w}{\partial x} + \Phi\frac{\dot{g}(\tau)}{g^2(\tau)}\lambda(\bar{S}_w)\frac{\partial S}{\partial x} = 0. \quad (3.2)$$

The independence of  $\tau$  in the coefficients in (3.2) implies we need to solve

$$g(\tau) = C^* \frac{\dot{g}(\tau)}{g^2(\tau)} \quad \text{for a } C^* \neq 0,$$

with general form of the solution

$$g(\tau) = \left( \frac{1}{g^2(\tau_0)} - \frac{2}{C^*}(\tau - \tau_0) \right)^{-\frac{1}{2}}.$$

**4. Model specification.** We use two main models for the capillary pressure  $p_c$  (as described in [3]):

$$\text{Brooks-Corey} \quad p_c(S_w) = p_d S_e^{-\frac{1}{\lambda}} \quad \text{for } p_c \geq p_d \quad (4.1)$$

$$\text{Van Genuchten} \quad p_c(S_w) = \frac{1}{\alpha} \left( S_e^{-\frac{1}{m}} - 1 \right)^{\frac{1}{n}} \quad \text{for } p_c > 0 \quad (4.2)$$

with parameters  $n$ ,  $m$ ,  $\lambda$  and  $\alpha$ , effective saturation  $S_e$  given by

$$S_e = \frac{S_w - S_{wr}}{1 - S_{wr}}$$

and residual wetting saturation  $S_{wr}$ , with relevant relative permeability coefficients  $k_{ri}$

$$\text{Burdine} \quad k_{rw}(S_w) = S_e^{\frac{2+3\lambda}{\lambda}} \quad (4.3)$$

$$k_{rn}(S_w) = (1 - S_e)^2 \left( 1 - S_e^{\frac{2+\lambda}{\lambda}} \right) \quad (4.4)$$

$$\text{Mualem} \quad k_{rw}(S_w) = S_e^\varepsilon \left[ 1 - \left( 1 - S_e^{\frac{1}{m}} \right)^m \right]^2 \quad (4.5)$$

$$k_{rn}(S_w) = (1 - S_e)^\gamma \left( 1 - S_e^{\frac{1}{m}} \right)^{2m} \quad (4.6)$$

where the parameter  $\lambda$  is an empirical Brooks-Corey's model constant from (4.1), other parameters  $\varepsilon$  and  $\gamma$  are closely connected with the pore structure and parameter  $m$  is the same as in Van Genuchten's model (4.2). Generally  $m = 1 - \frac{1}{n}$ ,  $\varepsilon = \frac{1}{2}$  and  $\gamma = \frac{1}{3}$ . Burdine's model is used together with Brooks-Corey's and Mualem's with Van Genuchten's model.

Permeability  $k_\alpha$  is then given by

$$k_\alpha(S_w) = k_0 k_{\alpha r}(S_w). \quad (4.7)$$

where the soil permeability  $k_0$  is characterising the specific soil (medium).

**5. Numerical solution.** As an alternative, we study the following one-dimensional transport problem

$$\Phi \frac{\partial S_w}{\partial t} = -q_t \frac{df}{dS_w} \frac{\partial S_w}{\partial x} + \frac{\partial}{\partial x} \left( D \frac{\partial S_w}{\partial x} \right) \quad \text{in } [0, +\infty] \times [0, L], \quad (5.1)$$

with

$$\begin{aligned} S_w &= S_w(t, x), \\ f &= f(S_w) = \frac{1}{1 + \frac{k_n(S_w) \mu_w}{k_w(S_w) \mu_n}}, \\ D &= D(S_w) = -\frac{1}{1 + \frac{k_n(S_w) \mu_w}{k_w(S_w) \mu_n}} \frac{k_n(S_w)}{\mu_2} \frac{dp_c}{dS_w}(S_w). \end{aligned}$$

The boundary and initial conditions are

$$S_w(t, L) = S_i, \quad (5.1.bc1)$$

$$S_w(t, 0) = S_0, \quad (5.1.bc2)$$

$$S_w(0, x) = S_i. \quad (5.1.ic)$$

The parameters used in the numerical and analytical computations are listed in Table 5.1.

Brooks-Corey & Burdine :	$\lambda = 2, \quad p_d = 2 \text{ Pa}$
Van Genuchten & Mualem :	$\alpha = 0.37 \text{ Pa}^{-1}, \quad n = 4.37$
common constants and parameters:	$S_{wr} = 0.01, \quad \Phi = 0.3,$ $\mu_w = \mu_n = 0.001 \text{ kg m}^{-1} \text{ s}^{-1},$ $k_0 = 10^{-10} \text{ m}^2$

TABLE 5.1

Values used in analytical and numerical computation are mainly taken from [3]. Parameters for the Van Genuchten model and the Brooks-Corey model pertain to same physical conditions.

The solution of (5.1)  $S_w = S_w(t, x)$  is compared to the solution given by (2.6).

A choice of the grid  $\omega_h = \{x_i | x_i = ih; i = 0, \dots, m; h = \frac{L}{m}\}$  leads to a discrete problem to find a grid-function  $u(t) : \omega_h \rightarrow R$  which approximates the solution  $S_w(t, x)$  of the problem (5.1). Its components  $u_i(t)$  resolve a system of  $(m - 1)$  ordinary differential equations (where there is used backward difference in the term replacing  $\frac{df}{dS_w}$ )

$$\frac{\partial u_i}{\partial t} = -\frac{q_t}{\Phi} \frac{f(u_i) - f(u_{i-1})}{h} + \frac{1}{\Phi} \frac{D_{i+\frac{1}{2}}(u_{i+1} - u_i) - D_{i-\frac{1}{2}}(u_i - u_{i-1})}{h^2} \quad i = 1, \dots, m - 1 \quad (5.2)$$

$$u_0(t) = S_0$$

$$u_m(t) = S_i$$

where  $D_{i\pm\frac{1}{2}}$  is defined by

$$D_{i+\frac{1}{2}} = D\left(\frac{u_{i+1} + u_i}{2}\right)$$

$$D_{i-\frac{1}{2}} = D\left(\frac{u_i + u_{i-1}}{2}\right)$$

with an initial condition

$$u_i(0) = S_i \quad \text{for } i = 1, \dots, m. \quad (5.3)$$

The problem (5.2) can be written in the form

$$\begin{aligned} \frac{\partial u}{\partial t} &= A(t, u) \quad \text{on } \langle 0, +\infty \rangle \\ u(0) &\equiv S_i \end{aligned} \quad (5.4)$$

The Runge-Kutta 4<sup>th</sup> order schema is used to resolve the problem (5.4) as in [1] (note that the time step is denoted by  $\tau$  and discrete time by  $t_n = n\tau$ ,  $n = 0, 1, 2, \dots$ ).

$$\begin{aligned} u(t_{n+1}) &= u(t_n) + \frac{\tau}{6}(\kappa_1 + 2\kappa_2 + 2\kappa_3 + \kappa_4) \quad n \in N_0 \\ \kappa_1 &= A(t_n, u) \\ \kappa_2 &= A(t_{n+\frac{1}{2}}, u + \frac{1}{2}\tau\kappa_1) \\ \kappa_3 &= A(t_{n+\frac{1}{2}}, u + \frac{1}{2}\tau\kappa_2) \\ \kappa_4 &= A(t_{n+1}, u + \tau\kappa_3) \end{aligned}$$

**5.1. Results.** In this section we present the numerical and quasi-analytical results obtained using this numerical scheme. It is obvious from the figures below that this numerical scheme is convenient to use as an numerical extension for the quasi-analytical procedure by McWhorter-Sunada.

The numerical solution is compared to the semi-analytical solution in the first series (Figures 5.1 to 5.4). The choice of the input saturation  $S_0$  is restricted only for values not too close to 1.00 because the iteration process of the equation (2.6) was found out not to be convergent for values close to 1.00.

The dependency of  $A$  on the prescribed value of  $S_0$  is demonstrated in Table 5.2.

$S_0$	0.3	0.5	0.7	0.9
$A_{Van\ Genuchten}$	0.479	1.440	3.227	7.239
$A_{Brooks-Corey}$	0.384	1.251	2.740	6.039

TABLE 5.2

The dependency of  $A$  on the prescribed value of  $S_0$ . The order of values of  $A$  is  $10^{-5}$ .

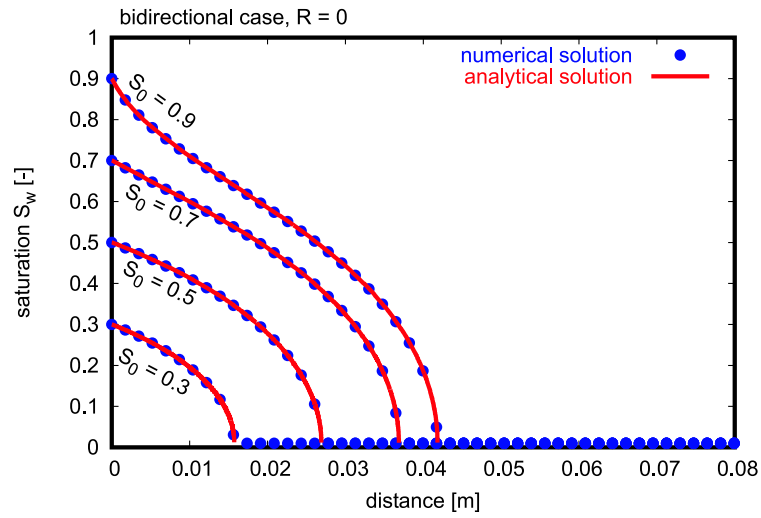


FIG. 5.1. Comparison of the numerical to the analytical solution using the Van Genuchten model. The numerical solution is obtained using a grid of 1000 nodes with a timestep of 0.01 s.

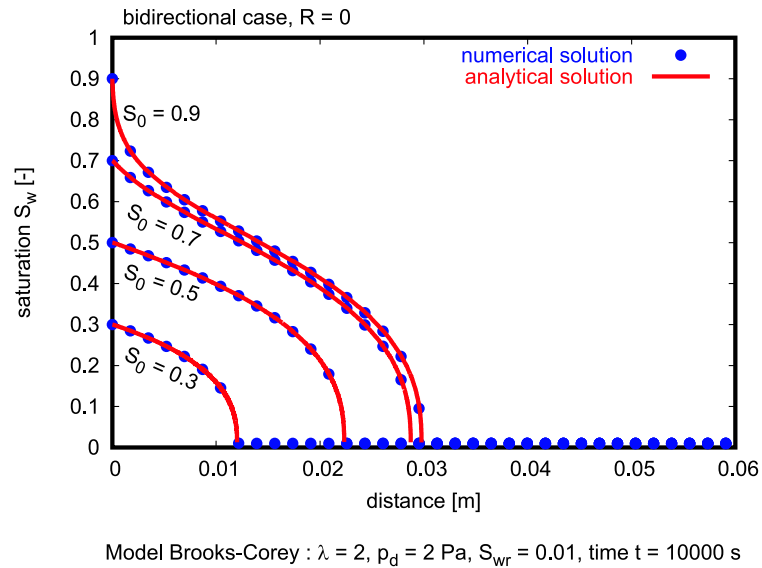


FIG. 5.2. Comparison of the numerical to the analytical solution using the Brooks-Corey model. The numerical solution is obtained using a grid of 1000 nodes with a timestep of 0.01 s.



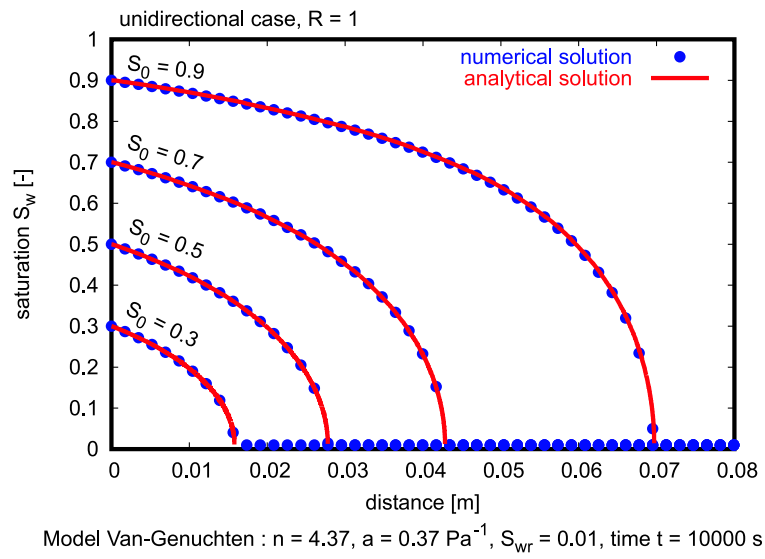


FIG. 5.3. Comparison of the numerical to the analytical solution using the Van Genuchten model. The numerical solution is obtained using a grid of 1000 nodes with a timestep of 0.01 s.

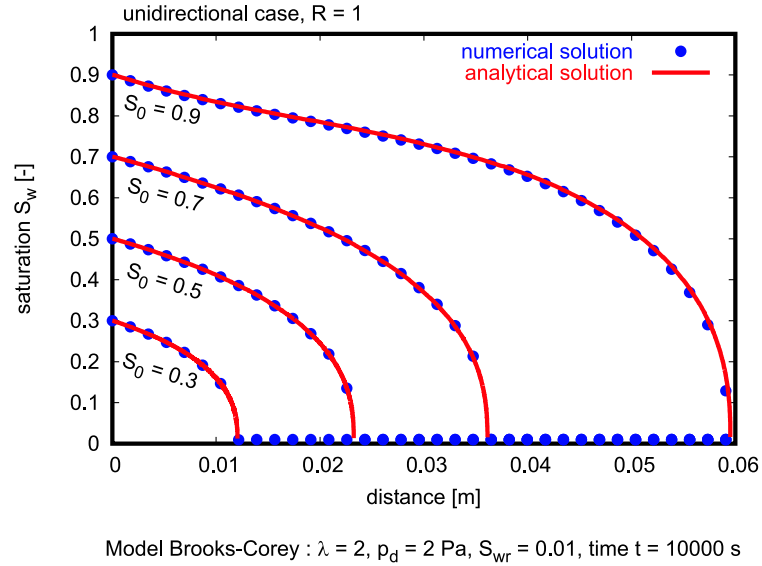
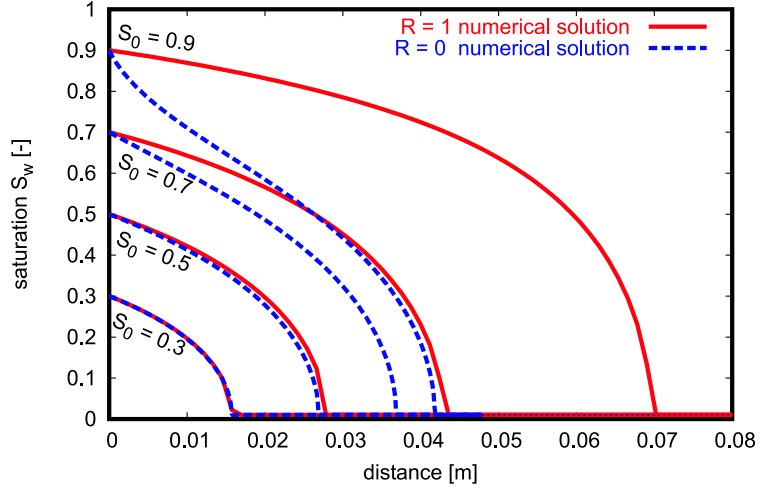


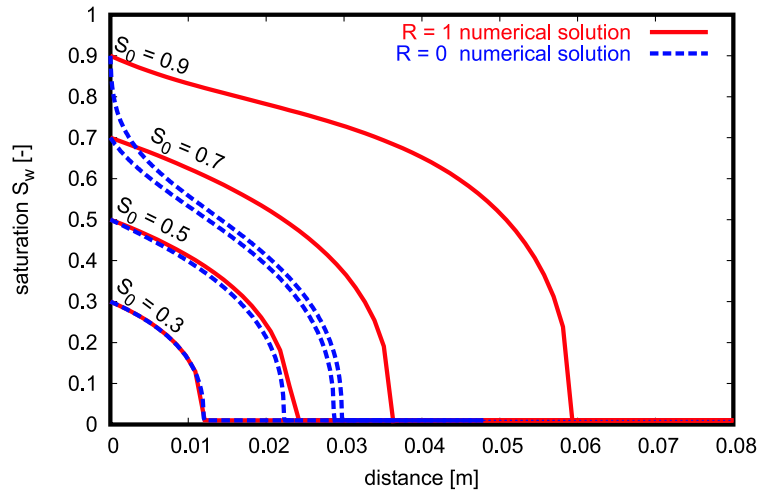
FIG. 5.4. Comparison of the numerical to the analytical solution using the Brooks-Corey model. The numerical solution is obtained using a grid of 1000 nodes with a timestep of 0.01 s.

Figures 5.5 and 5.6 present an interesting phenomenon in the comparison of the unidirectional and bidirectional displacement. Both curves agree up to certain level of  $S_0$  and then, as the value of  $S_0$  increases, the unidirectional displacement is faster as expected.



Model Van-Genuchten :  $n = 4.37$ ,  $\alpha = 0.37 \text{ Pa}^{-1}$ ,  $S_{wr} = 0.01$ , time  $t = 10000 \text{ s}$

FIG. 5.5. Comparison of the unidirectional and the bidirectional displacement using the Van-Genuchten model. The numerical solution is obtained using a grid of 1000 nodes with a timestep of 0.01 s.



Model Brooks-Corey :  $\lambda = 2$ ,  $p_d = 2 \text{ Pa}$ ,  $S_{wr} = 0.01$ , time  $t = 10000 \text{ s}$

FIG. 5.6. Comparison of the unidirectional and the bidirectional displacement using the Brooks-Corey model. The numerical solution is obtained using a grid of 1000 nodes with a timestep of 0.01 s.

**5.2. Suggestion to generalisation of the input.** In this section we present some ideas concerning the form of the input flux  $q_0(t)$ . We used some functions with

the same value at  $t = 0$  (except the first case). Results using our numerical scheme are presented in Figures 5.7 to 5.11. Values of  $A$  were based on preceding computations (see the Table 5.2) : for the Van Genuchten model,  $A = 7 \cdot 10^{-5}$  and for the Brooks-Corey model  $A = 6 \cdot 10^{-5}$ . Each result was obtained on the grid of 100 nodes with a timestep of 0.01 s and finaltime of 10000 s.

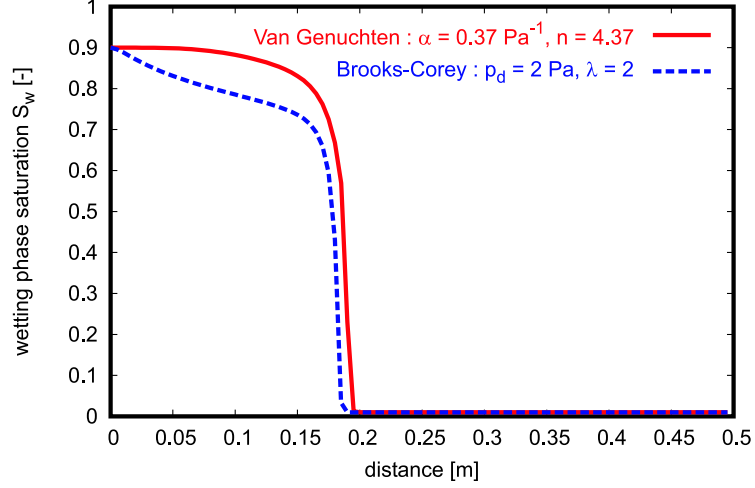


FIG. 5.7. Firstly, the numerical scheme was tested with a little modified input flux function  $q_0(t) = A t^{-\frac{1}{3}}$ .

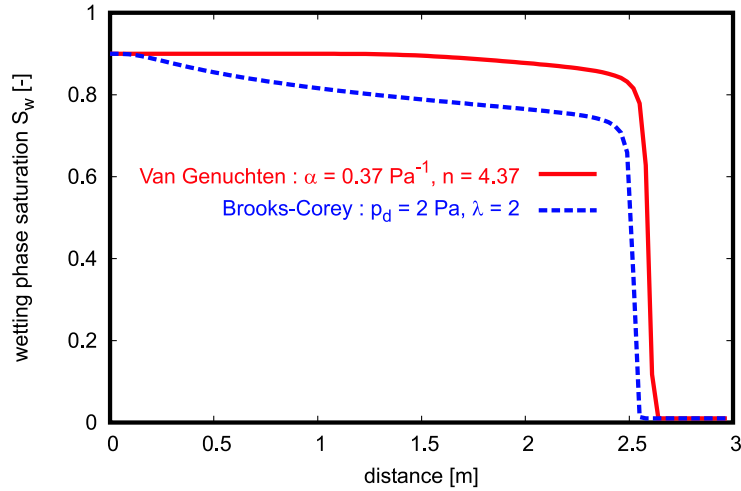


FIG. 5.8. In this case, the input flux function is constant  $q_0(t) = A$ .

**6. Conclusion.** The numerical scheme seems to be convenient for solving this class of problems even if it is impossible to find the quasi-analytical integral solution. Figures presented in Section 5.1 demonstrated that the numerical solution of the equation (1.7) equals to the benchmark solution, i.e. the semi-analytical solution. Consequently, we can introduce some new input fluxes and compute the solution of

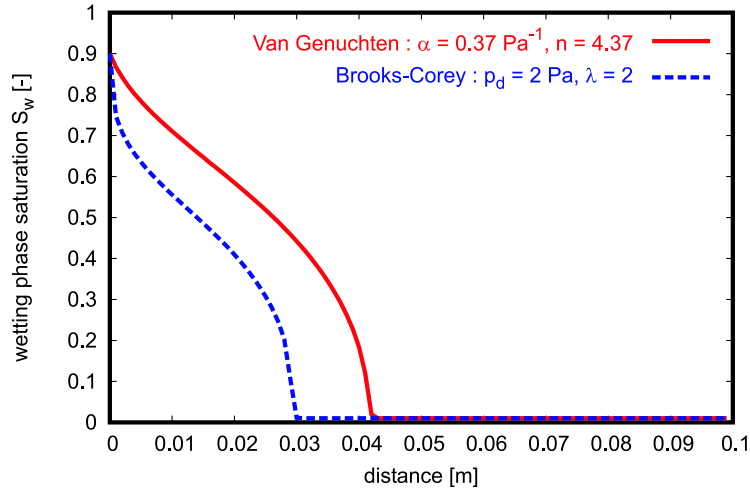


FIG. 5.9. In this case, the input flux function is constant only for a certain period of time.  $q_0(t) = A$  for  $t < 1000$  s else  $q_0(t) = 0$ .

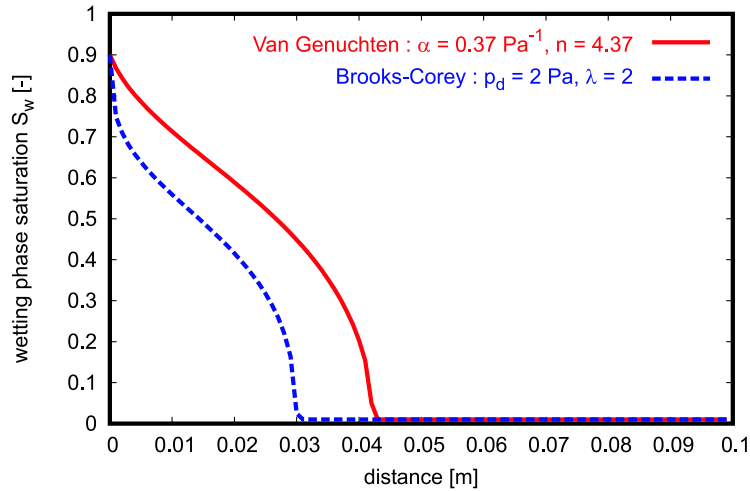


FIG. 5.10. The input flux function is  $q_0(t) = \frac{A}{t+1}$ . Curves seem to be similar to Figure 5.9, but it is only a coincidence.

the (1.7) using the verified numerical scheme as was shown in Section 5.2. There were not obtained any limitations concerning the shape of the input flux function yet.

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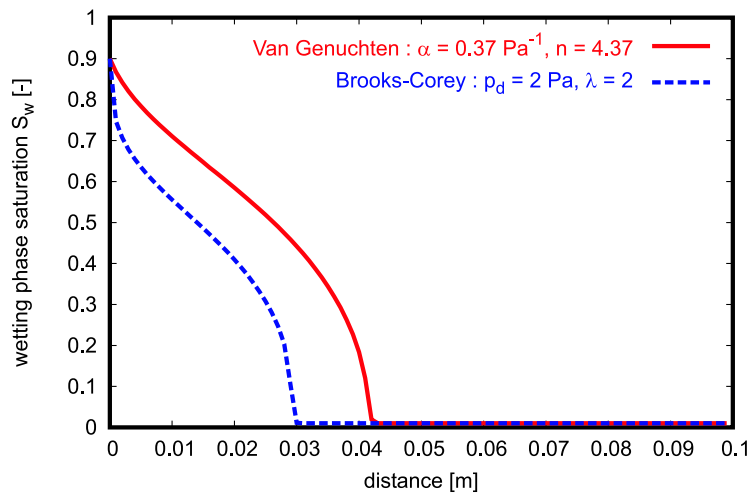


FIG. 5.11. The input flux function is  $q_0(t) = A e^{-t}$ .

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