NUMERICAL SIMULATION OF UNSATURATED FLOW IN POROUS MEDIA USING A MASS-CONSERVATIVE MODEL

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Abstract. *Water flow into unsaturated porous media is governed by the Richards' partial differential equation expressing the mass conservation law and the Darcy′s law. This equation may be written in three standard forms: the "h-based" form, the "θ-based" form, and the "mixed" form. Numerical aproximations based on different forms of this one-dimensional nonlinear equation can lead to significantly different results for unsaturated flow problems. In the h-based form generate poor results characterized by large mass balance errors and erroneous estimates of infiltration depth; whereas on the mixed form the mass is perfectly conserved, improving the accuracy of the results without requiring any additional computational effort. However, it is shown to be insufficient to guarantee good numerical solutions. In the present paper, the Richards' equation is modeled in mixed form discretized by finite differences techniques using a backward Euler time-marching coupled with modified Picard method, and arithmetical mean in estimating of the hydraulic conductivity (K) between neighbors points of the mesh. Starting from this model, simulations were made to Dirichlet and Neumann boundary conditions, soil initially very dry and types of soil with different permeability. Besides, were tested interblocks weighting for estimating of K using experimental data and comparing them with quasi-analytical solution.*

Keywords. *Porous media, Unsaturated flow, Richards' Equation, Finite difference, Infiltration*

1. Introduction

The water unsaturated zone of the earth's crust remains an enigma to scientific understanding and technological management. This zone, also called vadose zone, is a region of the underground limited at its top by the soil surface and below by the ground water table, where happened many physical phenomena such as: infiltration, evaporation, groundwater recharge, soil moisture storage and others. Prediction of fluid movement in unsaturated porous media is an important problem in many branches of science and engineering, such as the soil mechanics, the fluid mechanics, the agricultural engineering, the environmental engineering and others.

The equations that govern this phenomenon are Darcy's law and the mass conservation law. The unsaturated flow involves a two-phase flow of air and water, however only the flow of the water has been considered, where the air phase is continuous and is at atmospheric pressure, and it does not affect the dynamics of the water phase. The media is treated as isotropic and homogeneous, the flow is supposed one-dimensional and transient, the water density varies only with capillary pressure, and the thermal and salinity effects are neglected; thus the fluid motion is assumed to obey the classical Richards' equation.

2. Background

Numerical simulation of unsaturated flow has a significant history in the fields of soil science and groundwater hydrology. General overviews and thorough reviews of the literature may be found in the works of Nielsen et al. (1986) and Milly (1988). Almost all unsaturated flow simulations use either the h-based form of Richards' equation or the θ-based form. A variety of finite difference and finite element solution techniques have been used with each of these equation forms (Freeze, 1971; Neumann, 1973; Narasimhan and Witherspoon, 1976; Haverkamp et al., 1977; Hayhoe, 1978; Haverkamp and Vauclin, 1979; van Genuchten, 1980 and Huyakorn et al., 1984).

Therefore later, Allen and Murphy (1986) and Celia et al. (1987) used a mixed form of Richards' equation to derive numerical solution algorithms. These algorithms used collocation approximations in space, with Celia et all using an alternating-direction version. Allen and Murphy called their approximation a "quasi-Newton" method while Celia et al. referred to the method as a "modified Picard" method. Both demonstrated excellent mass balance in their numerical solutions. Zarba (1988) used the modified Picard iteration method with both finite difference and finite element approximations in space and demonstrated perfect mass balance. However, conservation of mass is shown to be insufficient to guarantee good numerical solutions. For infiltration into dry soils finite element approximations produce oscillatory solutions even while conserving mass (Celia et al., 1990).

Recently, Ross and Bristow (1990) used the Kirchhoff transformation to simulate water flow, however this procedure increased the computational effort. Srivastava and Yeh (1991) proposed an analytical solution using exponential function to linearize the Richards' equation. Zaidel and Russo (1992) used an asymptotic weighting scheme based on the behavior asymptotic of the hydraulic conductivity function. Gottardi and Venutelli (1993) presented a program, which integrates the three standard forms of this equation using finite difference and finite element

techniques. Finally, Huang et al. (1996) proposed a new convergence criterion for the modified Picard iteration method to improve the computational efficient of the algorithm of Celia et al. (1990).

The purpose of this paper is to present a versatile numerical model which is able to solve the one-dimensional Richards' equation with an accurate mass balance and which converges rapidly to the theoretically correct solution. The numerical model is able to handle short duration infiltration and is relatively easy to implement.

3. Governing partial differential equation

The governing equation may be written in several forms, where the dependent variable will be the pressure head $h(z,t)$ [L] or moisture content $\theta(z,t)$ [L³/L³], and the constitutive relationships between θ and h allow for conversion of one form into the other.

Three standard forms of the unsaturated flow equation may be identified: the "h-based" form, the "θ-based" form, and the "mixed" form. These equations are written as

H-based form

$$C(h)\frac{\partial h}{\partial t} = \frac{\partial}{\partial z}\left[K(h)\frac{\partial h}{\partial z}\right] - \frac{\partial K(h)}{\partial z}$$ (1)

θ-based form

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z}\left[D(\theta)\frac{\partial \theta}{\partial z}\right] - \frac{\partial K(\theta)}{\partial z}$$ (2)

Mixed form

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z}\left[K(\theta)\frac{\partial h}{\partial z}\right] - \frac{\partial K(\theta)}{\partial z}$$ (3)

where $K(h)$ or $K(\theta)$.[L/T] is the unsaturated hydraulic conductivity, $C(h)=d\theta/dh$ [1/L] is the moisture capacity, $D(\theta)=K(\theta)/C(\theta)$ [L²/T] is the unsaturated diffusivity and z denotes the vertical coordinate assumed positive downward.

The terms on the left side of Eq. (1), (2) and (3) describe the effects of draining and filling pores, so statement in terms of the temporal change in moisture content is more appropriate than description via the pressure. In other words, the term $(d\theta/dh)\partial h/\partial t$ is more appropriately written in its simpler form: $\partial\theta/\partial t$.

On the right side of Eq. (1), (2) and (3), it noted that the spatial derivative of the hydraulic head is used to describe the driving force for fluid movement. This is the most direct mathematical statement of the fact that head differences do indeed supply the energy required to move fluid. Specification of the hydraulic conductivity as a function of the pressure head, $K(h)$, is, however, not directly representative of the underlying physics. It is water-filled pores which facilitate transmission of water through a porous medium. The fact that, in modeling water behavior in the unsaturated zone, is secondary to the underlying physics of the flow, because water content and pressure are directly related. Consequently, the hydraulic conductivity, formally, should be expressed in terms of the moisture content, $K(\theta)$. Besides, $K(h)$ typically exhibits hysteresis, whereas in $K(\theta)$ is generally less pronounced (Nielsen et al., 1996).

Hence, the most direct mathematical expression of the physics of unsaturated flow, given the considerations above, is the mixed form presented in the Equation (3).

It was considered the problem of solving for equations above given the following initial and boundary conditions:

Dirichlet type (constant h or θ):

$$\begin{cases} h(z,0) = h_{initial}, & 0 < z < L \\ h(0,t) = h_0, & t > 0 \\ h(L,t) = h_{initial}, & t > 0 \end{cases}$$ (4)

Neumann type (constant flux):

$$\begin{cases} h(z,0) = h_{initial}, & z \neq 0 \\ h(0,0) = h_0 \\ h(L,t) = h_{initial}, & t > 0 \\ q(0,t) = q_0, & t > 0 \end{cases}$$ (5)

4. Numerical approach

In this section, the numerical approximation used in the model for solving three forms of the Richards' equation is given. The numerical discretization of these three partial differential equations by finite difference method (FD) leads to a tridiagonal nonlinear set of equation, which can be written in matrix form as

$$
\begin{bmatrix}
\beta_1^m & \gamma_1^m & 0 & 0 & 0 & \gg & \gg & 0 & 0 & 0 \\
\alpha_2^m & \beta_2^m & \gamma_2^m & 0 & 0 & \gg & \gg & 0 & 0 & 0 \\
0 & \alpha_3^m & \beta_3^m & \gamma_3^m & 0 & \gg & \gg & 0 & 0 & 0 \\
0 & 0 & \alpha_4^m & \beta_4^m & \gamma_4^m & \gg & \gg & 0 & 0 & 0 \\
0 & 0 & 0 & \alpha_5^m & \beta_5^m & \gg & \gg & 0 & 0 & 0 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \gg & \vdots & \vdots & \vdots \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\
0 & 0 & 0 & 0 & 0 & \gg & \gg & \beta_{N-2}^m & \gamma_{N-2}^m & 0 \\
0 & 0 & 0 & 0 & 0 & \gg & \gg & \alpha_{N-1}^m & \beta_{N-1}^m & \gamma_{N-1}^m \\
0 & 0 & 0 & 0 & 0 & \gg & \gg & 0 & \alpha_N^m & \beta_N^m
\end{bmatrix}
\begin{bmatrix}
\delta_1^{m+1} \\
\delta_2^{m+1} \\
\delta_3^{m+1} \\
\delta_4^{m+1} \\
\delta_5^{m+1} \\
\vdots \\
\vdots \\
\delta_{N-2}^{m+1} \\
\delta_{N-1}^{m+1} \\
\delta_N^{m+1}
\end{bmatrix}
=
\begin{bmatrix}
R_1^m \\
R_2^m \\
R_3^m \\
R_4^m \\
R_5^m \\
\vdots \\
\vdots \\
R_{N-2}^m \\
R_{N-1}^m \\
R_N^m
\end{bmatrix}
\tag{6}
$$

where the coefficients $\alpha_i^m, \beta_i^m, \gamma_i^m$, and R_i^m (i = 1,2,...,N; where N is the number of nodes) are nonlinear function of the variables h or θ . The dependent variables are the increment of the variables h or θ for passing from the iteration level m to the iteration level m+1 and are written as

$$
\delta_j^{m+1} = h_j^{m+1} - h_j^m \qquad \text{or} \qquad \delta_j^{m+1} = \theta_j^{m+1} - \theta_j^m, \qquad (j = i-1, i, i+1)
\tag{7}
$$

However the superscript n refer to time, where $\Delta t = t^{n+1} - t^n$. Then, the Eq. (7) can be rewritten as

$$
\delta_j^{n+1,m+1} = h_j^{n+1,m+1} - h_j^{n+1,m} \qquad \text{or} \qquad \delta_j^{n+1,m+1} = \theta_j^{n+1,m+1} - \theta_j^{n+1,m}, \qquad (j = i-1, i, i+1)
\tag{8}
$$

In this paper, the set of nonlinear algebraic Equations (6) is solved by using a standard fully implicit Picard iterative technique and the algorithm of Thomas. The models for the three forms of Richards's equation are given in the following.

H-based approximation

The standard FD approximation for the h-based form (HFD) of the Richards' equation (1) obtained by a backward Euler method for temporal discretization is

$$
C_i^{n+1,m} \frac{h_i^{n+1,m+1} - h^n}{\Delta t} = \frac{K_{i-1/2}^{n+1,m}}{(\Delta z)^2}\left(h_{i-1}^{n+1,m+1} - h_i^{n+1,m+1}\right) + \frac{K_{i+1/2}^{n+1,m}}{(\Delta z)^2}\left(h_{i+1}^{n+1,m+1} - h_i^{n+1,m+1}\right) - \frac{K_{i+1/2}^{n+1,m} - K_{i-1/2}^{n+1,m}}{\Delta z}
\tag{9}
$$

where $K_{i\pm1/2}^{n+1,m}$ indicate the interblock hydraulic conductivities. Substituting the increment of pressure head at two subsequent iteration levels, Eq. (8), in the equation above we obtain

$$
C_i^{n+1,m} \frac{\delta_i^{n+1,m+1}}{\Delta t} + \frac{K_{i-1/2}^{n+1,m}}{(\Delta z)^2}\left(\delta_{i-1}^{n+1,m+1} - \delta_i^{n+1,m+1}\right) + \frac{K_{i+1/2}^{n+1,m}}{(\Delta z)^2}\left(\delta_{i+1}^{n+1,m+1} - \delta_i^{n+1,m+1}\right) = \frac{K_{i-1/2}^{n+1,m}}{(\Delta z)^2}\left(h_{i-1}^{n+1,m} - h_i^{n+1,m}\right) +
$$
$$
+ \frac{K_{i+1/2}^{n+1,m}}{(\Delta z)^2}\left(h_{i+1}^{n+1,m} - h_i^{n+1,m}\right) - \frac{K_{i+1/2}^{n+1,m} - K_{i-1/2}^{n+1,m}}{\Delta z} - C_i^{n+1,m} \frac{h_i^{n+1,m} - h_i^n}{\Delta t} \equiv (R_i^{n+1,m})
\tag{10}
$$

where $(R_i^{n+1,m})$ is defined as the residual associated with the Picard iteration. Upon convergence in iteration, both $(R_i^{n+1,m})$ and the difference in iteration, Equation (8), approach zero. The Equation (10) can be put in the form of Equation (6) where

$$\begin{cases} \alpha_i^{n+1,m} = -\dfrac{K_{i-1/2}^{n+1,m}}{(\Delta z)^2}; \\[3mm] \beta_i^{n+1,m} = \dfrac{C_i^{n+1,m}}{\Delta t} + \dfrac{K_{i-1/2}^{n+1,m}}{(\Delta z)^2} + \dfrac{K_{i+1/2}^{n+1,m}}{(\Delta z)^2}; \\[3mm] \gamma_i^{n+1,m} = -\dfrac{K_{i+1/2}^{n+1,m}}{(\Delta z)^2}; \\[3mm] R_i^{n+1,m} = \dfrac{K_{i-1/2}^{n+1,m}}{(\Delta z)^2}\left(h_{i-1}^{n+1,m} - h_i^{n+1,m}\right) + \dfrac{K_{i+1/2}^{n+1,m}}{(\Delta z)^2}\left(h_{i+1}^{n+1,m} - h_i^{n+1,m}\right) - \dfrac{K_{i+1/2}^{n+1,m} - K_{i-1/2}^{n+1,m}}{\Delta z} - C_i^{n+1,m}\dfrac{h_i^{n+1,m} - h_i^n}{\Delta t} \end{cases} \tag{11}$$

θ-based approximation

The standard FD approximation for the θ-based form (TFD) of the Richards' equation (2) obtained by a backward Euler method for temporal discretization is

$$\frac{\theta_i^{n+1,m+1} - \theta^n}{\Delta t} = \frac{D_{i-1/2}^{n+1,m}}{(\Delta z)^2}\left(\theta_{i-1}^{n+1,m+1} - \theta_i^{n+1,m+1}\right) + \frac{D_{i+1/2}^{n+1,m}}{(\Delta z)^2}\left(\theta_{i+1}^{n+1,m+1} - \theta_i^{n+1,m+1}\right) - \frac{K_{i+1/2}^{n+1,m} - K_{i-1/2}^{n+1,m}}{\Delta z} \tag{12}$$

where $D_{i\pm1/2}^{n+1,m}$ indicate the interblock unsaturated diffusivities. Substituting the increment of moisture content at two subsequent iteration levels, Eq. (8), in the equation above we obtain

$$\frac{1}{\Delta t} + \frac{D_{i-1/2}^{n+1,m}}{(\Delta z)^2}\left(\delta_{i-1}^{n+1,m+1} - \delta_i^{n+1,m+1}\right) + \frac{D_{i+1/2}^{n+1,m}}{(\Delta z)^2}\left(\delta_{i+1}^{n+1,m+1} - \delta_i^{n+1,m+1}\right) = \frac{D_{i-1/2}^{n+1,m}}{(\Delta z)^2}\left(\theta_{i-1}^{n+1,m} - \theta_i^{n+1,m}\right) +$$

$$+ \frac{D_{i+1/2}^{n+1,m}}{(\Delta z)^2}\left(\theta_{i+1}^{n+1,m} - \theta_i^{n+1,m}\right) - \frac{K_{i+1/2}^{n+1,m} - K_{i-1/2}^{n+1,m}}{\Delta z} - \frac{\theta_i^{n+1,m} - \theta_i^n}{\Delta t} \equiv (R_i^{n+1,m}) \tag{13}$$

The Equation (13) can be put in the form of Eq.(6) where

$$\begin{cases} \alpha_i^{n+1,m} = -\dfrac{D_{i-1/2}^{n+1,m}}{(\Delta z)^2}; \\[3mm] \beta_i^{n+1,m} = \dfrac{1}{\Delta t} + \dfrac{D_{i-1/2}^{n+1,m}}{(\Delta z)^2} + \dfrac{D_{i+1/2}^{n+1,m}}{(\Delta z)^2}; \\[3mm] \gamma_i^{n+1,m} = -\dfrac{D_{i+1/2}^{n+1,m}}{(\Delta z)^2}; \\[3mm] R_i^{n+1,m} = \dfrac{D_{i-1/2}^{n+1,m}}{(\Delta z)^2}\left(\theta_{i-1}^{n+1,m} - \theta_i^{n+1,m}\right) + \dfrac{D_{i+1/2}^{n+1,m}}{(\Delta z)^2}\left(\theta_{i+1}^{n+1,m} - \theta_i^{n+1,m}\right) - \dfrac{K_{i+1/2}^{n+1,m} - K_{i-1/2}^{n+1,m}}{\Delta z} - \dfrac{\theta_i^{n+1,m} - \theta_i^n}{\Delta t} \end{cases} \tag{14}$$

Mixed approximation

The standard FD for the mixed-based form (MFD) of the Richards' equation (3) obtained by a backward Euler method for temporal discretization is

$$\frac{\theta_i^{n+1,m+1} - \theta^n}{\Delta t} = \frac{K_{i-1/2}^{n+1,m}}{(\Delta z)^2}\left(h_{i-1}^{n+1,m+1} - h_i^{n+1,m+1}\right) + \frac{K_{i+1/2}^{n+1,m}}{(\Delta z)^2}\left(h_{i+1}^{n+1,m+1} - h_i^{n+1,m+1}\right) - \frac{K_{i+1/2}^{n+1,m} - K_{i-1/2}^{n+1,m}}{\Delta z} \tag{15}$$

where $K_{i\pm1/2}^{n+1,m}$ indicate the interblock hydraulic conductivities. The key to the method is expansion of $\theta_i^{n+1,m+1}$ in a truncated Taylor series with respect to h, about the expansion point $h_i^{n+1,m}$, namely,

$$\theta_i^{n+1,m+1} = \theta_i^{n+1,m} + \frac{d\theta}{dh}\bigg|^{n+1,m}(h^{n+1,m+1} - h^{n+1,m}) + O(\delta^2) \tag{16}$$

If all terms higher than linear are neglected in Eq.(16), and this equation is substituted into Eq. (15), it results

$$\left(\frac{1}{\Delta t}C_i^{n+1,m}\right)\delta_i^{n+1,m} + \frac{\theta_i^{n+1,m+1} - \theta^n}{\Delta t} = \frac{K_{i-1/2}^{n+1,m}}{(\Delta z)^2}\left(h_{i-1}^{n+1,m+1} - h_i^{n+1,m+1}\right) +$$

$$+ \frac{K_{i+1/2}^{n+1,m}}{(\Delta z)^2}\left(h_{i+1}^{n+1,m+1} - h_i^{n+1,m+1}\right) - \frac{K_{i+1/2}^{n+1,m} - K_{i-1/2}^{n+1,m}}{\Delta z} \tag{17}$$

Substituting the increment of pressure head at two subsequent iteration levels, Eq. (8), in the equation above we obtain

$$C_i^{n+1,m}\frac{\delta_i^{n+1,m}}{\Delta t} + \frac{K_{i-1/2}^{n+1,m}}{(\Delta z)^2}\left(\delta_{i-1}^{n+1,m+1} - \delta_i^{n+1,m+1}\right) + \frac{K_{i+1/2}^{n+1,m}}{(\Delta z)^2}\left(\delta_{i+1}^{n+1,m+1} - \delta_i^{n+1,m+1}\right) = \frac{K_{i-1/2}^{n+1,m}}{(\Delta z)^2}\left(h_{i-1}^{n+1,m} - h_i^{n+1,m}\right) +$$

$$+ \frac{K_{i+1/2}^{n+1,m}}{(\Delta z)^2}\left(h_{i+1}^{n+1,m} - h_i^{n+1,m}\right) - \frac{K_{i+1/2}^{n+1,m} - K_{i-1/2}^{n+1,m}}{\Delta z} - \frac{\theta_i^{n+1,m} - \theta_i^n}{\Delta t} \equiv (R_i^{n+1,m}) \tag{18}$$

where $(R_i^{n+1,m})$ is defined as the residual associated with the Modified Picard iteration (Celia et al. ,1990). The Equation (18) can be rewritten and the coefficients of Equation (6) become

$$\begin{cases} \alpha_i^{n+1,m} = \dfrac{K_{i-1/2}^{n+1,m}}{(\Delta z)^2}; \\[4mm] \beta_i^{n+1,m} = \dfrac{C_i^{n+1,m}}{\Delta t} + \dfrac{K_{i-1/2}^{n+1,m}}{(\Delta z)^2} + \dfrac{K_{i+1/2}^{n+1,m}}{(\Delta z)^2}; \\[4mm] \gamma_i^{n+1,m} = -\dfrac{K_{i+1/2}^{n+1,m}}{(\Delta z)^2}; \\[4mm] R_i^{n+1,m} = \dfrac{K_{i-1/2}^{n+1,m}}{(\Delta z)^2}\left(h_{i-1}^{n+1,m} - h_i^{n+1,m}\right) + \dfrac{K_{i+1/2}^{n+1,m}}{(\Delta z)^2}\left(h_{i+1}^{n+1,m} - h_i^{n+1,m}\right) - \dfrac{K_{i+1/2}^{n+1,m} - K_{i-1/2}^{n+1,m}}{\Delta z} - \dfrac{\theta_i^{n+1,m} - \theta_i^n}{\Delta t} \end{cases} \tag{19}$$

4.1. Discretization of boundary conditions

In the present paper, Dirichlet and Neumann boundary conditions are allowed. For each, the Eq. (6) is modified in the top and bottom node. In the Dirichlet condition, where the pressure head are known, the coefficients $\alpha_2^m, \alpha_n^m, \gamma_1^m, \gamma_{n-1}^m, R_1^m$ and R_n^m of matrix of Eq. (6) are equaled to zero, and β_1^m and β_n^m are equaled to unity. On the other hand, the Neumann condition, where the flux is known on the top node, is given by imposing

$$q = -\left(K\frac{\partial h}{\partial z} + K\right) \qquad \text{or} \qquad q = -\left(D\frac{\partial \theta}{\partial z} + D\right) \tag{20}$$

where q is the prescribed flux. So doing, the coefficients in Eq. (6) for the first block are obtained from those of the generic internal ith-block as follows

$$\begin{cases} \alpha_1^m = 0; \\[2mm] \beta_1^m \quad \text{from} \quad \beta_i^m \quad \text{by putting:} \quad K_{1-1/2}^m = 0 \quad \text{or} \quad D_{1-1/2}^m = 0; \\[2mm] \gamma_1^m \quad \text{from} \quad \gamma_i^m; \\[2mm] R_1^m \quad \text{from} \quad R_i^m \quad \text{by putting:} \quad \dfrac{K_{1-1/2}^m}{(\Delta z)^2}\left(h_0^m - h_1^m\right) + \dfrac{K_{1-1/2}^m}{\Delta z} = 0 \quad \text{or} \quad \dfrac{D_{1-1/2}^m}{(\Delta z)^2}\left(\theta_0^m - \theta_1^m\right) + \dfrac{D_{1-1/2}^m}{\Delta z} = 0. \end{cases} \tag{21}$$

4.2. Estimating of interblock nonlinear functions

The application of finite difference operator provokes the problem of approximating the $i\pm1/2$ level in space, referred to as "weighting" necessary for the determination of interblock hydraulic conductivity values $K_{i\pm1/2}$ or unsaturated diffusivity values $D_{i\pm1/2}$. Different weighting formulas for estimating interblock quantities from the available grid point are proposed (Haverkamp and Vauclin, 1979):

Arithmetic mean

$$K_{i\pm1/2} = \frac{K_i + K_{i\pm1}}{2} \quad \text{and} \quad D_{i\pm1/2} = \frac{D_i + D_{i\pm1}}{2} \tag{22}$$

Harmonic mean

$$K_{i\pm1/2} = \frac{2K_i K_{i\pm1}}{K_i + K_{i\pm1}} \quad \text{and} \quad D_{i\pm1/2} = \frac{2D_i D_{i\pm1}}{D_i + D_{i\pm1}} \tag{23}$$

Geometric mean

$$K_{i\pm1/2} = \sqrt{K_i K_{i\pm1}} \quad \text{and} \quad D_{i\pm1/2} = \sqrt{D_i D_{i\pm1}} \tag{24}$$

Upstream method

$$\begin{cases} K_{\mp1/2} = K_{i\mp1} \quad \text{or} \quad D_{i\mp1/2} = D_{i\mp1} \quad \text{if} \quad h_{i\mp1} > h_i \quad \text{or} \quad \theta_{i\mp1} > \theta_i \\ K_{\mp1/2} = K_i \quad \text{or} \quad D_{i\mp1/2} = D_i \quad \text{if} \quad h_{i\mp1} < h_i \quad \text{or} \quad \theta_{i\mp1} < \theta_i \end{cases} \tag{25}$$

4.3. Evaluation of mass balance error

One measure of a numerical simulator is its ability to conserve global mass over the domain of interest. Adequate conservation of global mass is a necessary but not sufficient condition for acceptability of a numerical simulator (Celia et al., 1990). To measure the ability of the simulator to conserve mass, let a mass balance measure be defined as follows

$$MB(t) \equiv \frac{\text{total additional mass in the domain}}{\text{total net flux into the domain}} \tag{26}$$

where the additional mass is measured with respect to the initial mass in the system. For the finite difference approximation with Dirichlet boundary conditions, this is evaluated as

$$MB(t^{n+1}) = \frac{\sum_{i=1}^{N-1} (\theta_i^{n+1} - \theta_i^0)(\Delta z)}{\sum_{j=1}^{n+1} \left\{ K_{1/2}^j \left[\frac{h_2^j - h_1^j}{\Delta z} + 1 \right] - K_{N-1/2}^j \left[\frac{h_N^j - h_{N-1}^j}{\Delta z} + 1 \right] \right\}(\Delta t)} \tag{27}$$

where N is the number of nodes whose coordinates are $\{z_1, z_2, ..., z_N\}$, and constant nodal spacing Δz is assumed. The global mass balance error is calculated by

$$MBE(\%) = 100 \left| 1 - MB(t) \right| \tag{28}$$

5. Experimental constitutive relationships

The constitutive relationships between θ, h and K are given by experimental functions, that describe the soil properties. In this paper, three usual types of constitutive relationships $K=K(h)$ and $\theta = \theta(h)$ can be used to characterize the different soil. The first and second type were used by Haverkamp et al. (1977) for a sand and for the Yolo light clay, whereas the third type have been used by van Genuchten (1980) to model the Glendale clay loam. The numerical values of the parameters for these types of soils are given in Table 1 (Gottardi and Venutelli, 1993).

Type 1

$$K(h) = K_s \frac{A}{A + |h|^\phi}; \qquad \theta(h) = \frac{\lambda(\theta_s - \theta_r)}{\lambda + |h|^\psi} + \theta_r \qquad (29)$$

Type 2

$$K(h) = K_s \frac{A}{A + |h|^\phi}; \qquad \theta(h) = \frac{\lambda(\theta_s - \theta_r)}{\lambda + (\ln|h|)^\psi} + \theta_r \qquad (30)$$

Type 3

$$K(S_e) = K_s S_e^{1/2} \left[1 - \left(1 - S_e^{1/\mu}\right)^\mu\right]^2; \qquad \theta(S_e) = S_e(\theta_s - \theta_r) + \theta_r \qquad (31)$$

where

$$S_e(h) = \left[1 + (\rho h)^\eta\right]^{-\mu}; \qquad \mu = 1 - \eta^{-1} \qquad (32)$$

where $A, \phi, \lambda, \psi, \eta, \mu$ are dimensionless parameters, ρ [L^{-1}] is a measure of the pore size density function, θ_s [L^3/L^3] is the moisture content at saturated conditions, θ_r [L^3/L^3] is the residual moisture content and S_e is effective saturation.

Table 1. Parameter values for three types of soil.

Soil	Type	K_s (cm/s)	A	λ	ϕ	ψ	ρ (cm^{-1})	η	θ_s (cm^3/cm^3)	θ_r (cm^3/cm^3)
Sand	1	$9.44 \ 10^{-3}$	$1.18 \ 10^6$	$1.61 \ 10^6$	4.47	3.96	-	-	0.287	0.075
Yolo	2	$1.23 \ 10^{-5}$	$1.25 \ 10^2$	$7.39 \ 10^2$	1.77	4.00	-	-	0.495	0.124
Glendale	3	$1.52 \ 10^{-4}$	-	-	-	-	$1.04 \ 10^{-2}$	1.395	0.469	0.106

6. Test cases and results

Infiltration simulations in homogeneous soils are present in the following test cases. The simulations were carried out using the theory described in the previous sections where all three numeral approximations methods were used.

Test case 1

This test case consists of infiltration into an unsaturated soil (Sand, type 1 - Table 1) column with a depth L=120 cm. The simulation was made at Dirichlet conditions, with a depth interval $\Delta z = 1.0$ cm and a time step varying from $\Delta t = 10^{-6}$ s during 4000 s (1,11 h). The arithmetical mean was used for estimating K. The results of this simulation are in the Fig. 1, and the initial and boundary conditions for this test were

$$\begin{cases} h(z,0) = -100 \text{ cm} \quad (\theta = 0.07903 \text{ cm}^3/\text{cm}^3), \quad 0 < z < 120 \\ h(0,t) = -20 \text{ cm} \quad (\theta = 0.269 \text{ cm}^3/\text{cm}^3), \qquad t > 0 \\ h(120,t) = -100 \text{ cm}, \quad t > 0 \end{cases} \qquad (33)$$

Test case 2

This test case consists of infiltration into an unsaturated soil (Glendale clay loam, type 3 - Table 1) column with a depth L=200cm. The simulation was made at Neumann conditions, with a depth interval $\Delta z = 2.0$ cm and a time step varying from $\Delta t = 10^2$ s during 1.5×10^5 s (41.67 h). The arithmetical mean was used for estimating K. The results of this simulation are in the Fig. 2, and the initial and boundary conditions for this test were

$$\begin{cases} h(z,0) = -600 \text{ cm}, \quad z \neq 0 \\ h(0,0) = -20 \text{ cm} \quad (\theta = 0.4579 \text{ cm}^3/\text{cm}^3) \\ h(200,t) = -600 \text{ cm} \quad (\theta = 0.2781 \text{ cm}^3/\text{cm}^3), \quad t > 0 \\ q(0,t) = 0.0001 \text{ cm/s}, \qquad t > 0 \end{cases} \qquad (34)$$
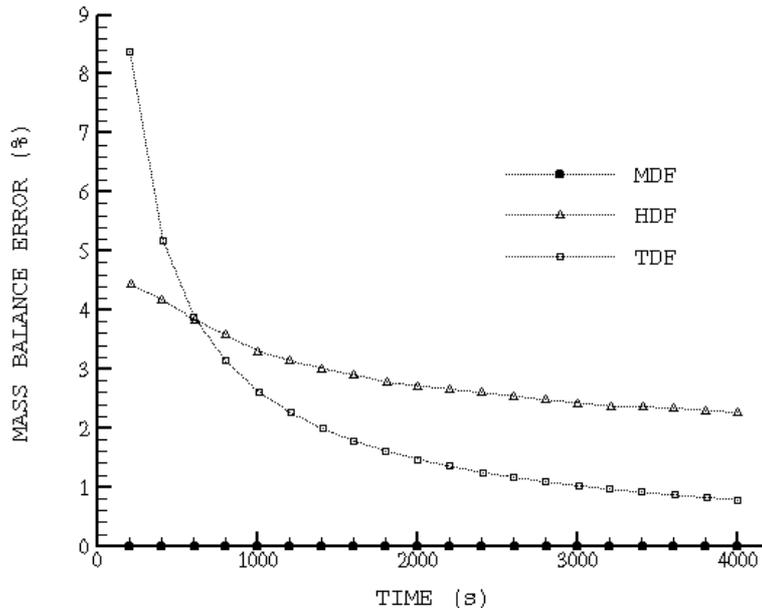
Figure 1. Mass balance error versus time for MDF, HDF and TDF methods.
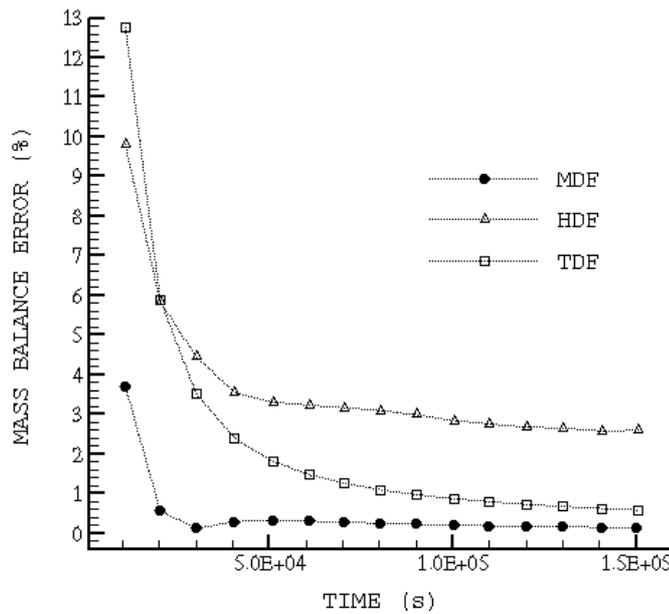
Figure 2. Mass balance error versus time for MDF, HDF and TDF methods.

Test case 3

This test case consists of infiltration into an unsaturated soil (Sand, type 1 – Table 1) column with a depth L=100cm. The simulation was made at Dirichtet conditions, with a depth interval $\Delta z = 1.0$ cm and a time step varying from $\Delta t = 10^{-6}$ s during 3600s (1.0 h). The MDF method with four types for estimating K were used and compared with the quasi-analytical solution by Philip (Kaverkamp et al., 1977). The results of this simulation are in the Fig. 3, and the initial and boundary conditions for this test were

$$\begin{cases} h(z,0) = -61.50 \text{ cm} \quad (\theta = 0.100 \text{ cm}^3 / \text{cm}^3), \quad 0 < z < 100 \\ h(0,t) = -20.73 \text{ cm} \quad (\theta = 0.267 \text{ cm}^3 / \text{cm}^3), \qquad t > 0 \\ h(100,t) = -61.50 \text{ cm}, \quad t > 0 \end{cases} \qquad (35)$$

Test case 4

This test case consists of infiltration into an unsaturated soil (Yolo light clay, type 2 – Table 1) column with a depth L=220cm. The simulation was made at Dirichtet conditions, with a depth interval $\Delta z = 1.0$ cm and a time step varying from $\Delta t = 10^2$ s during 4.0×10^6 s (46.3 days). The MDF method and geometric mean for estimating K was used and compared with the quasi-analytical solution by Philip. The results of this simulation are in the Fig. 4, and the initial and boundary conditions for this test were

$$\begin{cases} h(z,0) = -600.0 \text{ cm} \quad (\theta = 0.2376 \text{ cm}^3/\text{cm}^3), \quad 0 < z < 220 \\ h(0,t) = -1.0 \text{ cm} \quad (\theta = \theta_s = 0.4950 \text{ cm}^3/\text{cm}^3), \quad t > 0 \\ h(220,t) = -600.0 \text{ cm}, \quad t > 0 \end{cases} \qquad (36)$$
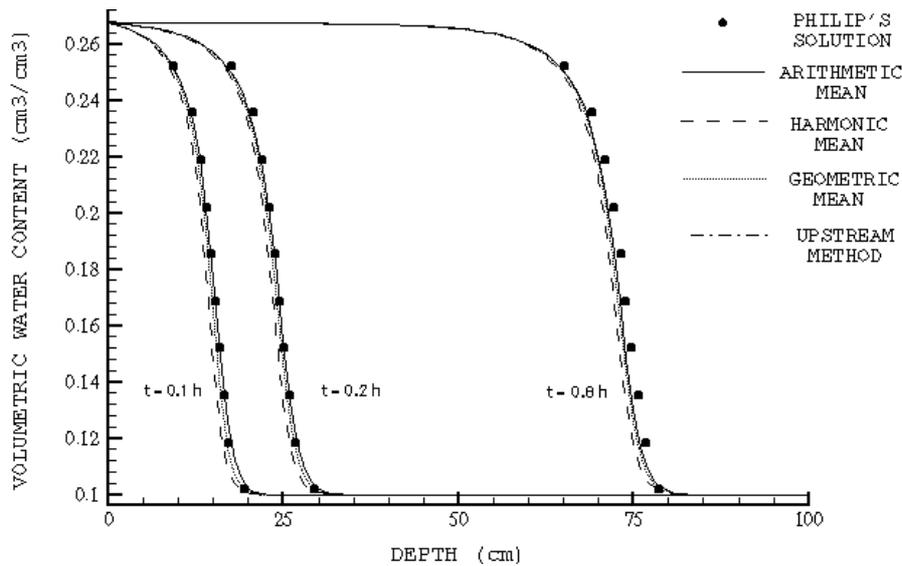
Figure 3. Moisture profiles at times: 0.1, 0.2 and 0.8 h for four estimates of K using MDF method and for quasi-analytical solution by Philip.
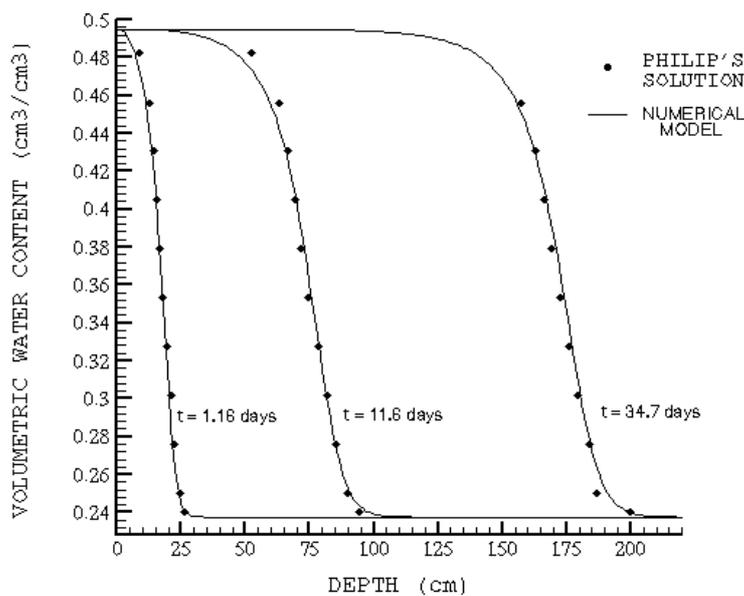
Figure 4. Moisture profiles at times: 1.16, 11.6 and 34.7 days for the most mass-conservative numerical model and for quasi-analytical solution by Philip.

7. Conclusion

The comparison of the performance of the methods on the basis of mass-balance errors, the analyze of estimating nonlinear functions and the confirmation of the validity of numerical solution were allowed by tests cases.

In the test cases one and two were shown that the mixed form of the Richards' equation is the most mass conservative solution for sandy and loamy soils, besides Dirichlet and Neumann boundary conditions. This result checks in another way the solution obtained by Celia et al. (1990). In the test case three it was shown that the geometric mean is the solution more accurate in the estimate of the hydraulic conductivity in relation to the quasi-analytic solution by Philip. And, in the last test case was used the best results of the test case previous to model a well-known clay of the literature (Yolo light clay). The good match obtained confirms the validity of the numerical method employed.

However, this paper presented a versatile numerical model which was able to solve the one-dimensional Richards' equation with an accurate mass balance and which converges rapidly to the theoretically correct solution. The numerical model was able to handle short duration infiltration and was relatively easy to implement.

One reason why research continues on the numerical solution of the Richards' equation is the computational time needed to achieve to accurate solution for heterogeneous soils with abruptly changing wetness conditions. Therefore, this work will continue in search of those objectives.

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