18th Brazilian Congress of Thermal Sciences and Engineering
November 16-20, 2020 (Online)

ENC-2020-0476
SOLUTION OF THE RICHARDS EQUATION IN A SOIL PROFILE WITH TWO LAYERS USING THE METHOD OF LINES

Diego Sousa Lopes
Augusto Cezar Cordeiro Jardim
Graduate Program in Chemical Engineering, Institute of Technology, Federal University of Pará
diegosousa.eng@gmail.com, augustojardim@gmail.com

Diego Cardoso Estumano
School of Biotechnology, Institute of Biological Sciences, Federal University of Pará
dcestumano@ufpa.br

Emanuel Negrão Macêdo
João Nazareno Nonato Quaresma
School of Food Engineering, Graduate Program in Chemical Engineering, Graduate Program in Process Engineering, Graduate Program in Natural Resources Engineering in the Amazon, Institute of Technology, Federal University of Pará
enegrao@ufpa.br, quaresma@ufpa.br

Abstract. *This work aims to solve the Richards Equation for the unidirectional flow of water through horizontal layers, using a single domain approach. We propose a mathematical formulation in which a transition function is introduced between the layers to smooth the discontinuity present in the interface. The Method of Lines (MOL), together with the Finite Volume Method (FVM), is used to solve the problem. The verification of the obtained solution was accomplished through the comparison with those results of Srivastava and Yeh (1991). In all the studied cases, we performed convergence analyses, and numerical experiments were carried out to analyze the influences of the parameter* K_s*, the saturated hydraulic conductivity. The results show a good agreement with the values obtained in the literature. The model for water content through the single domain approach can deal with the discontinuity at the interface, and that the proposed transition function was adequate to solve the problem.*

Keywords: *method of lines, Richards equation, layered soils*

1. INTRODUCTION

The phenomena of infiltration and water movement in the soil are essential topics for the study of the hydrological cycle of vegetated ecosystems. In such events, the ability to infer soil moisture and its interaction with vegetation has outstanding practices in hydrology, climate science, engineering, agriculture, and ecosystem management (Broadbridge, 2017).

Generally, the process of infiltration into the soil is represented by the Richards Equation (RE) (Richards, 1931), which presents an advection-diffusion term derived from mass conservation, which generalizes Darcy's law to the saturated flow in a porous medium (Farthing and Ogden, 2017; Berardi *et al*., 2018).

Soils, in turn, are inherently heterogeneous at different scales. Usually, soil profiles show layered characteristics, which have a major influence on the phenomenon of infiltration, redistribution of water moisture in the soil, and groundwater recharge. Hydraulic properties, such as unsaturated hydraulic conductivity, can vary in magnitude in different layers, while soil moisture can be discontinued at the interfaces between layers, these characteristics pose challenges to the numerical solution of the Richards equation (Zha et al., 2019).

Generally, the θ-form of the RE, where θ represents the water content, is not used for layered soils, as there is a discontinuity in the value of θ at the interface. Hills et al. (1989) were the first to develop a numerical solution for the θ-form for infiltration into a layered soil profile.

However, the non-iterative numerical model employed an explicit scheme, which requires very small-time steps. Matthews et al. (2004) solved this problem using the Method of Lines (MOL), in which the moisture discontinuity is considered by an explicit algorithm, applying the principle of mass conservation to develop the boundary conditions at the interface, introducing fictitious points at the interface, in which the boundary conditions were treated using explicit and iterative approximations (Zha et al., 2019). Other works have continued to improve the stability of the model using implicit algorithms to explain the discontinuity of the soil moisture as follows in the references in (Zha et al., 2013; Berardi et al., 2017; Berardi et al., 2019).

In the present work, a model for infiltration of water into a two-layers soil is presented, with a single domain approach proposing a transition function at the interface between layers. Dependence on hydraulic conductivity is given by the Gardner model (1958). Therefore, the mathematical formulation for the Richards equation in the θ-form accounts for the effects of saturated hydraulic conductivity on the diffusive flow of water that are also evaluated in terms of the soil wetting cycle hydraulic pressure exerted along of soil profile. A transition function at the interface allows deal with the problem in a single domain formulation, which contributes to the literature from a methodological perspective. Although more recent works have used the method of lines (MOL) as a solution methodology for the Richards equation, they do not use such a single domain approach (Mathews et al., 2005; Zha et al., 2013; Berardi and Vurro, 2016; Farthing and Ogden, 2017; Zha et al., 2019).

In light of this, the MOL approach was used together with a Finite Volume Method (FVM) scheme, proposing a mesh with elements of centered volumes, with a regular and fixed mesh to numerically solve the system of Partial Differential Equations (PDEs) of the proposed model. The application of MOL results in a system of Ordinary Differential Equations (ODEs), which are solved numerically through the development of a code based on the FORTRAN 90/95 programming language. Numerical results were generated for water content (θ) and hydraulic pressure (h), showing the wetting front across the two-layers soil profile, at different times, and the effects of saturated hydraulic conductivity varying along of the soil profile. The solution methodology used in this work will be validated with the results obtained in the literature.

2. MATHEMATICAL FORMULATION

The Richards equation that governs the vertical, unidimensional, and transient flow in unsaturated soils in the *θ*-form is given by (Matthews et al., 2004):

$$\frac{\partial q}{\partial t} = \frac{\partial}{\partial z}\left[D(q)\frac{\partial q}{\partial z} \right] - \frac{\partial K(q)}{\partial z}, \qquad 0 < z < L, \quad t > 0 \tag{1}$$

$$q(z,0) = q_0(z), \qquad 0 \pounds z \pounds L \tag{2}$$

$$\frac{\P q(0,t)}{\P z} = \frac{K[q(0,t)] - q_s(t)}{D[q(0,t)]}, \qquad t > 0 \tag{3}$$

$$q(L,t) = q_s, \qquad t > 0 \tag{4}$$

Where $K(\theta)$ is the hydraulic conductivity, $D(\theta)$ is the hydraulic diffusivity of water in the soil, which follows the relationship, $D(\theta)=K(\theta)/C(\theta)$, where $C(\theta)=\mathrm{d}\theta/\mathrm{d}h$ is the water capacity of the ground and h is the hydraulic pressure, z is the vertical coordinate, defined as positive downwards, and t is the time.

The flow governed by Eq. (1) will be solved under the effect of a constant flow on the surface (q_s), and a saturated lower limit (θ_s), with the presence of continuous flow conditions at the interface between layers, with an initial condition $\theta_0(z)$, which is the steady-state solution of Eq. (1) in terms of θ with an infiltration rate q_I at the interface z=0.

2.1 Single domain formulation

It will be considering a horizontal porous layer (soil) of thickness L, with two layers L_1 and L_2. The phenomenon of hysteresis is neglected; that is, the parameters of the pore size distribution are assumed the same for the drainage cycles ($\alpha=\alpha_1=\alpha_2$) and moistening of the soil; for both layers, its value varies only according to the z position. The saturated hydraulic conductivity of the soil K_s is different and constant for both soil segments (see scheme in Fig. 1).

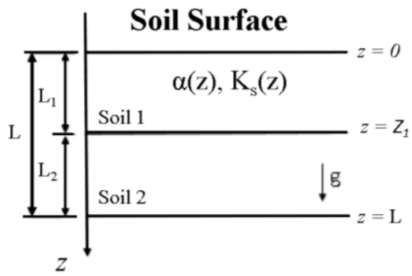

Figure 1. Layered soil profile.

The hypothesis of solving the problem of a double domain in a single one consists of combining the equations that govern the two regions in a unique set of equations valid for the entire *z*-coordinate. For this purpose, a transition function for K_s is proposed as

$$K_s(z) = (K_{s2} - K_{s1})\, f(z) + K_{s1} \tag{5}$$

where K_{s1} and K_{s2} are the saturated hydraulic conductivity of the soils 1 and 2, and $f(z)$ is a function that represents the transition coefficient expressed as follows

$$f(z) = \frac{1}{\left[1 + e^{-(z-Z_1)/(\omega \Delta Z)}\right]} \tag{6}$$

Where Z_1 is the interface position between layers and Δz is an interval between one point and another on the medium, and ω is a parameter of the transition, which is related to the amplitude of the transition curve. Equation (5) is proposed to make $K_s(z)$ continuous; this, in turn, is caused by impositions of capillary forces, called capillary barrier (Hills et al., 1989), which is the result of variation of the physical properties of each soil. Therefore, this function differs from other approaches to the Richards equation solution in that it treats the layers as being in a single domain, with the presence of a transition function at the interface between layers.

2.2 Hydraulic function and semi-analytical solution

An analytical solution for the one-dimensional transient infiltration in a two-layer soil profile was developed by Srivastava and Yeh (1991). This solution is valid for some forms of hydraulic functions and initial conditions, in the present work the dependence on the hydraulic conductivity and water content in hydraulic pressure (*h*) are described by the following relationships proposed by Gardner (1958).

$$K = K_s e^{\alpha h} \tag{7}$$

$$\theta = \theta_r + (\theta_s - \theta_r) e^{\alpha h} \tag{8}$$

and,

$$C = \frac{d\theta}{dh} = \alpha(\theta_s - \theta_r) e^{\alpha h} \tag{9}$$

Where θ_s and θ_r are the saturated and residual water content, K_s is the saturated hydraulic conductivity, and α is a pore size distribution parameter. Given the relation of Eq. (8) the hydraulic functions for the θ-form of the Richards equation are

$$K = K_s \left(\frac{\theta - \theta_r}{\theta_s - \theta_r} \right) \tag{10}$$

$$D = \frac{K}{C} = \frac{K_s}{\alpha(\theta_s - \theta_r)} \tag{11}$$

A semi-analytical solution for the single domain is developed, in which α is equivalent for both types of soils. The shape of the hydraulic functions results in C given by Eq. (9), i.e., a non-zero constant, therefore in the saturation, h=0. According to Matthews et al. (2004), when comparing a numerical solution with an analytical one for homogeneous soils that follow linear models, such as those given by Eqs. (10) and (11), there is no guarantee that this numerical precision will be preserved in non-homogeneous and more realistic soils. However, the present approach is a way of verifying that the boundary conditions at the interface are handled correctly.

The initial condition is a steady-state profile for the initial constant flow (q_I) in which the transition function is introduced into the solution, given by the following expression:

$$\theta(z) = \theta_r + (\theta_s - \theta_r) e^{\alpha(z-L)} \left[1 + \alpha q_I e^{\alpha L} \int_z^L \frac{e^{-\alpha z}}{K_s(z)} dz \right], \quad 0 \le z \le L \tag{12}$$

Equation (12) for $\theta(z)$ is a single-domain solution that can be generalized to N soil layers. The introduction of a transition function is used to smooth the discontinuity at the interfaces. A such solution is semi-analytical because the integral part is solved employing a numerical integrator. In the present work, we used the subroutine DQDAGS from the IMSL Library (2018).

3. SOLUTION METHODOLOGY

A procedure based on the MOL approach is developed to solve the proposed mathematical model. This methodology consists of replacing the spatial derivatives of the PDEs with algebraic approximations. Thus, only the time variable remains in the mathematical formulation, resulting in a system of ordinary differential equations (ODEs) integrated by any conventional numerical integrator (Özisik, 1993; Hamdi et al., 2007).

Equation (1) was discretized in finite volumes following the steps described in Maliska (2004). Therefore, the soil profile is divided into small volumes in the spatial *z*-direction; the diffusive term's interpolation was approximated by the upstream weighted method. The axial variable was divided into N intervals, as shown in Fig. 2, where $N_z=N_1+N_2$, (i.e., $N_1=Z_1/\Delta Z_1$, $N_2=(L-Z_1)/\Delta Z_1$), $N_z=L/\Delta Z_1$, and this procedure is valid for the nodes $1\leq z\leq N_z-1$. The soil surface is at $z=0$ (the node referenced as $i=0$), and the bottom of the soil column at $z=L$, (node $i=N_z$). As it deals with a single domain, the transition will take place at $z=N_1$, then the soil 1 changes instantly to soil 2. The point $i=0$ is part of a fictional volume in which is calculated by an implicit function of θ_0 .

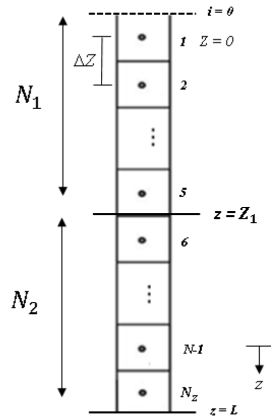

Figure 2. Scheme of the domain discretization.

The ODEs system, resulting from the application of the MOL procedure, is given by:

$$\frac{d\theta_i}{dt} = \frac{\Delta_i - \Gamma_i}{\Delta Z}, 1 \leq i \leq N_z, \ \ t > 0 \tag{13}$$

$$\theta_{i=0} = \theta_0(z), \ 0 \leq i \leq N_Z \tag{14}$$

$$D\left(\theta_i\right)\frac{\theta_{i+1}-\theta_i}{\Delta z/2} = K\left(\theta_i\right) - q_s, \ t>0, \ 1\leq i \leq N_Z \tag{15}$$

$$q_{N_z} = q_S, \ t>0 \tag{16}$$

where,

$$\Delta_i = D\left(\theta_e\right)\frac{\theta_2-\theta_1}{\Delta z} - (K(\theta_w)-q_s)\Big|_{w(i=0)} \tag{17}$$

$$\Gamma_i = K(\theta_e) - K\left(\theta_w\right), \theta_w = \theta_0 \tag{18}$$

$$\theta_0 = \theta_1 - \frac{\Delta Z}{2}\left(\frac{K(\theta_0)-q_s}{D(\theta_0)}\right) \tag{19}$$

The objective now is to compute the properties at the interface as a function of both soils. A grid is then developed where the interface between soils is coupled into a single mesh; thus, the application of MOL leads to a unique set of ODEs coupled through the boundary condition at the interface.

4. RESULTS AND DISCUSION

A computational code was developed in the FORTRAN 90/95 programming language to solve the system of ODEs given by Eqs. (13) to (19), resulting from the application of (MOL) to a uniform and regular grid. The subroutine DIVPAG from the IMSL Library (2018) was used to solve the initial value problem, where the user prescribed a relative error of 10^{-8}. The numerical result for the water content, θ, and hydraulic pressure, also called hydraulic potential, h, were calculated and compared with those from the works available in the literature.

The works of Matthews et al. (2004), and Srivastava and Yeh (1991) were used as references to obtain the values of the hydraulic parameters, where θ_s and θ_r, are 0.4 and 0.06, respectively. The initial water flow is taken as q_I=0.1 cm/h, and for t>0, an input flow given by q_s=0.9 cm/h is defined. Each layer's length is adopted as L_1=L_2=100 cm, and all simulations were performed for a final time of 100 h. Table 1 presents the input data, which are theoretical soils proposed by Srivastava and Yeh (1991). In this table, the values of K_s vary between layers, and the pore size distribution parameter α is constant for the cases analyzed.

Table 1. Soil parameters.

	α (cm^{-1})	**K_{s1} (cm/h)**	**K_{s2} (cm/h)**
Case 1	0.1	10	1
Case 2	0.1	1	10

A convergence analysis is performed to evaluate the computational performance of the solution methodology. Different values were tested for N_z (the number of points in the grid) in various positions in the soil profile by considering the times t=1h and t=100 h. The numerical values presented in Tabs. 2 and 3 refer to $\theta(z,t)$ distribution. Note that a good convergence is found near upper and lower boundaries, and for the intermediate positions, larger N_z values were needed. Therefore, N_z=400 was the value adopted to reach a full convergence with three significant digits and to simulate all the cases in the present work.

Table 2. Convergence analysis for t = 1h at different positions.

			***t*=1 h**		
***N*$_z$**	*z*=10 cm	*z*=95 cm	*z*=100 cm	*z*=105 cm	*z*=190 cm
50	0.0849	0.078	0.090	0.093	0.202
100	0.0849	0.079	0.092	0.097	0.204
200	0.0849	0.080	0.093	0.097	0.205
400	0.0849	0.081	0.092	0.095	0.206

Table 3. Convergence analysis for t = 100h at different positions.

			***t*=1 h**		
***N*$_z$**	*z*=10 cm	*z*=95 cm	*z*=100 cm	*z*=105 cm	*z*=190 cm
50	0.0906	0.174	0.303	0.273	0.376
100	0.0906	0.203	0.331	0.340	0.377
200	0.0906	0.226	0.347	0.364	0.378
400	0.0906	0.240	0.356	0.366	0.378

Figures 3 and 4 provide a comparison of the water content, θ, and hydraulic pressure, h. This comparative analysis is between the present MOL results for the diffusive flow of water in the soil against those analytical results of Srivastava and Yeh (1991). The solution obtained in terms of θ for the Richards equation is used to get the hydraulic pressure values through its relation given by Eq. (8) since the analytical solution provided by Srivastava and Yeh (1991) is in terms of the hydraulic pressure so that it can permit a comparison with those results from the analytical solution.

Figures 3 and 4 show the wetting and pressure profiles at different times along two layers of the soil. The present patterns present the effects of K_s on the grounds since it is a physical property representing the soil's hydraulic conductivity and can explain the speed that a given liquid passes through that medium (Libardi, 2005). A comparison between profiles in Figs. 3 and 4 show the effect of the position of a highly conductive layer on the spread of the wetting front. In Fig. 3, it can be seen that the infiltration is initiated in a high conductivity layer (i.e., K_{s1}>K_{s2}), since the wetting front when encountering a lower conductivity at the interface the hydraulic pressure tends to increase rapidly so that that moisture can move in a layer with less conductivity. On the other hand, in Fig. 4, the infiltration starts with a lower conductivity (i.e., $K_{s1}<K_{s2}$). When the wetting front reaches the interface with the layer that has a higher conductivity, the flow of moisture to this layer can be quickly dissipated.

Thus, according to the results also observed by Srivastava and Yeh (1991), the hydraulic gradient remains approximately constant, and the flow between layers behaves as continuous steady-state flows.

The comparison between the MOL solution and the analytical one proposed by Srivastava and Yeh (1991) provided excellent results. This warrant that the present work presented a viable and computationally efficient alternative. It offered a solution for the θ-form of the Richards equation with an approach of a single domain, where the employment of a transitive function at the interface permitted smooth discontinuity between layers.

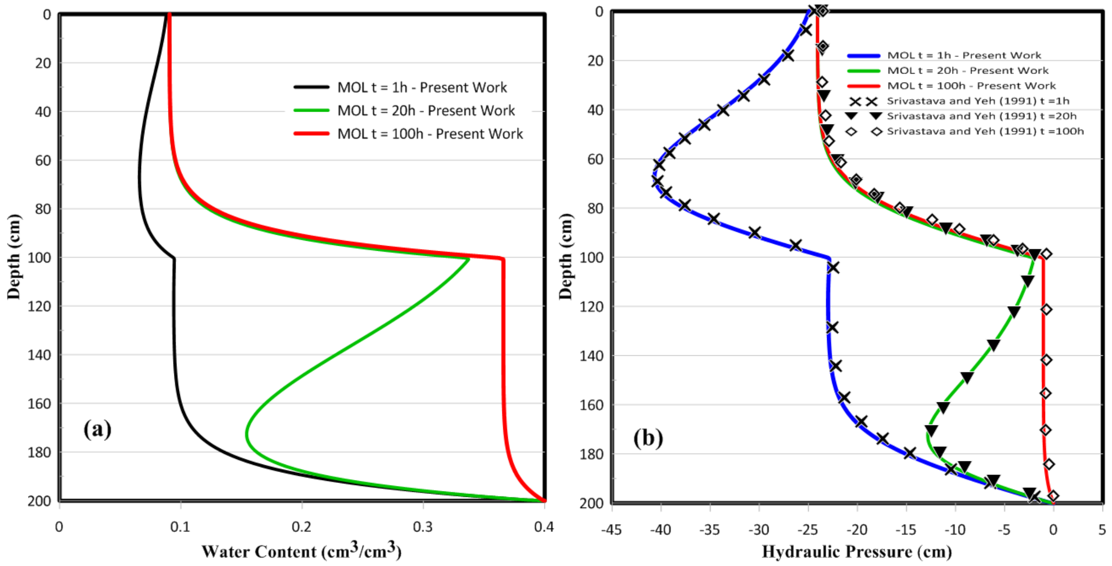

Figure 3. Water content and hydraulic pressure distributions for α=0.1 cm^{-1}, K_{s1}=10 (cm/h), K_{s2}=1 (cm/h), N_z=400, Δz=0.5 cm, ω=0.3, and times t=1 h, t=20 h and t=100h: (a) MOL solution for water content; (b) Comparison of the present MOL results with those of Srivastava and Yeh (1991) for the hydraulic pressure.

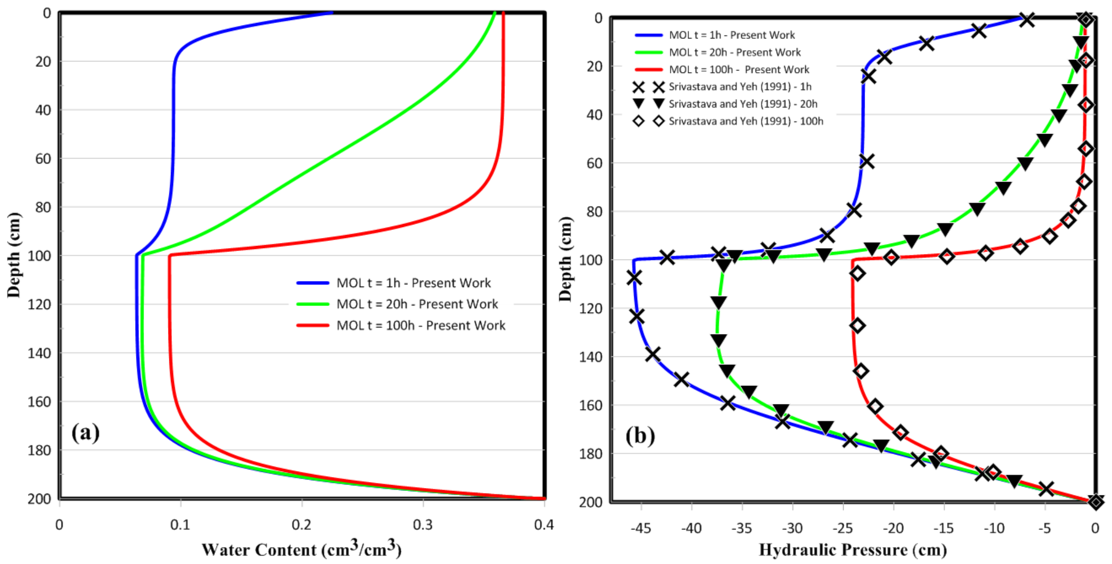

Figure 4. Water content and hydraulic pressure distributions for α=0.1 cm^{-1}, K_{s1}=1 (cm/h), K_{s2}=10 (cm/h), N_z=400, Δz=0.5 cm, ω=0.3, and times t=1 h, t=20 h and t=100h: (a) MOL solution for water content; (b) Comparison of the present MOL results with those of Srivastava and Yeh (1991) for the hydraulic pressure.

5. CONCLUSIONS

In this work, a theoretical study of the water infiltration process in layers was developed, in which the Richards equation was used to describe the mathematical formulation of the problem. A linear function for hydraulic conductivity was used as a strategy to overcome the problem of discontinuity at the interface between the soil layers. We applied the MOL approach with a scheme of FVM to obtain a system of ODEs that was numerically solved through code based on the FORTRAN 90/95 programming language using the DIVPAG subroutine from IMSL Library (2018). The excellent agreement of the present results with those in the literature demonstrated that the approach with a single domain used in this work was adequate to model the infiltration of water in a soil profile with two layers.

6. ACKNOWLEDGEMENTS

The authors would like to acknowledge the Coordenação de Aperfeiçoamento de Pessoal de Nível Superior (CAPES) for the financial support during the period of the M.Sc. studies of the author Diego Sousa Lopes.

7. REFERENCES

Berardi, M., Andrisani, A., Lopez, L., & Vurro, M., 2016. "A new data assimilation technique based on ensemble Kalman filter and Brownian bridges: An application to Richards' equation". Computer Physics Communications, Vol. 208, pp. 43-53.

Berardi, M., Difonzo, F., Notarnicola, F. and Vurro, M., 2018 "A transversal method of lines for the numerical modeling of vertical infiltration into the vadose zone". Applied Numerical Mathematics, Vol. 135, pp. 264-275.

Berardi, M., Difonzo, F., Vurro, M. and Lopez, L., 2017. "The 1D Richards' equation in two layered soils: a Filippov approach to treat discontinuities". Advances in Water Resources, Vol. 115, pp. 264-272.

Broadbridge, P., Daly, E. and Goard, J., 2017. "Exact solutions of the Richards equation with nonlinear plant-root extraction". Water Resources Research, Vol. 53, pp. 9679-9691.

Farthing, M.W. and Ogden, F.L., 2017. "Numerical solution of Richards' equation: a review of advances and challenges". Soil Science Society of America Journal, Vol. 81, pp. 1257-1269.

Gardner, W.R., 1958. "Some steady-state solutions of the unsaturated moisture flow equation with application to evaporation from a water table". Soil Science, Vol. 85, pp. 228-232.

Hamdi, S., Schiesser, W. and Griffiths, G., 2007. "Method of Lines". Scholarpedia, Vol. 2, pp. 2859.

Hills, R.G., 1989. "Modeling one-dimensional infiltration into very dry soils: 1. Model development and evaluation". Water Resources Research, Vol. 25, pp. 1259-1269.

IMSL® Fortran Numerical Library, 2018. Version 2018, Rogue Wave Software Inc., Boulder, USA.

Libardi, P.L., 2005. "Dinâmica da Água no Solo". Editora da Universidade de São Paulo.

Maliska, C.R., 2004. "Transferência de Calor e Mecânica dos Fluidos Computacional". LTC Eitora, Florianópolis, Brasil, 2nd Edtion.

Matthews, C.J., Braddock, R.D. and Sander, G.C., 2004. "Modeling flow through a one-dimensional multi-layered soil profile using the method of lines". Environmental Modeling & Assessment, Vol. 9, pp. 103-113.

Mathews, C.J., Cook, F.J., & Sander, G.C., 2005. "Handling the water content discontinuity at the interface between layered soils within a numerical scheme. Australian Journal of Soil Research". Australian Journal of Soil Research, Vol. 43, pp. 945-955.

Ozisik, M.N., 1993. "Heat Conduction". John Wiley, 2nd Edition.

Richards, L.A., 1931. "Capillary conduction of liquids through porous mediums". Physics, Vol. 1, pp. 318-333.

Srivastava, R. and Yeh, T.C.J., 1991. "Analytical solutions for one-dimensional, transient infiltration toward the water table in homogeneous and layered soils". Water Resources Research, Vol. 27, pp. 753-762.

Zha, Y., Shi, L., Ye, M., & Yang, J. 2013. "A generalized Ross method for two- and three-dimensional variably saturated flow". Advances in Water Resources, Vol. 54, pp. 67-77.

Zha, Y., Yang, J., Shi, L. and Song, X., 2013. "Simulating one-dimensional unsaturated flow in heterogeneous soils with water content-based Richards equation". Vadose Zone Journal, Vol. 12, pp. 1-13.

Zha, Y., Yang, J., Zeng, J., Tso, C-H.M., Zeng, W. and Shi, L., 2019. "Review of numerical solution of Richardson-Richards equation for variably saturated flow in soils". Wiley Interdisciplinary Reviews: Water, Vol. 6, pp. 1-23.

8. RESPONSIBILITY NOTICE

The authors are the only responsible for the printed material included in this paper.