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Sensitivity Analysis of Infiltration using a Mass Conservative Numerical Solution of Richards Equation

Choi, Hyun Il†

Assistant professional Scientist, Center for Atmospheric Science, Illinois State Water Survey, USA

Richards 방정식의 질량보존적 수치해석 해법에 의한 침투량의 민감도분석

최현일†

미국 일리노이주 수자원조사국 기상연구팀 연구원

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Abstract

Water flow into unsaturated soils is most often modeled by Richards equation consisting of the mass conservation law and Darcy's law. Three standard forms of Richards equation are presented as the head (Ψ)-based form, the moisture content (θ) based form, and the mixed form. Numerical solutions of these partial differential equations with highly nonlinear terms can cause poor results along with significant mass balance errors. The numerical solution based on the mixed form of Richards equation is known that the mass is perfectly conserved without any additional computational efforts. The aim of this study is to develop fully implicit numerical scheme of Richards equation for one-dimensional vertical unsaturated flow in homogeneous soils using the finite difference approximation, and then to perform sensitivity analysis of infiltration to the variations in the unsaturated soil properties and to different soil types.

keywords : Finite difference approximation, Fully implicit scheme, Infiltration, Richards equation, Unsaturated flow

1. Introduction

The unsaturated zone of subsurface is one of the important water resources for terrestrial hydrologic cycle where a complex water-redistribution mechanism exists, such as infiltration, evapotranspiration, groundwater recharge, water storage, and so on. The prediction of water movement in unsaturated soils is an important issue in many study fields such as terrestrial hydrology, soil mechanics, fluid mechanics, environmental engineering, etc.

Numerical models to simulate water flow in unsaturated porous media have been developed based on the solution of the Richards equation (Richards, 1931). There are alternative forms of the Richards equation which have either pressure head (Ψ) or moisture content (θ) as dependent variables of the equation. Since these equations contain highly nonlinear terms, a variety of finite difference and finite element schemes have been employed for each of these equation forms (Freeze, 1971; Haverkamp et al., 1977, 1979; Hayhoe, 1978; Huyakorn et al., 1984; Narasimhan et al., 1976; Neumann, 1973; van Genuchten, 1980). The numerical solutions based on the standard Ψ-based form of Richards equation usually lead to incorrect estimations of infiltration depth along with large mass balance errors (Celia et al., 1987; Milly, 1985). The θ-based form of Richards equation have demonstrated reliable mass balance accuracy (Haverkamp et al., 1977). However, this θ-based formulation has drawbacks in that moisture content is a discontinuous variable, and application of this scheme is restricted to unsaturated flow conditions. Numerical solutions based on the mixed form of Richards equation show the better mass conservative property than the results of standard Ψ-based form of Richards equation, while maintaining the advantages of the Ψ-based formulation (Allen et al., 1985; Celia et al., 1987, 1990).

In this study, it is assumed that the porous media is isotropic and homogeneous, and one-dimensional vertical water movement is dominant in the vadose zone. The lateral flow induced by topography, and the thermal and salinity effects are neglected. The objective of this study is to perform sensitivity analysis of infiltration to the variations in the unsaturated soil properties and to different soil types after developing the mass conservative numerical solution of Richards equation using the finite difference approximation.

† To whom correspondence should be addressed.
hichoi@uiuc.edu

2. Modeling of Richards Equation

2.1. Governing Equation

There are three standard forms of Richards equation for one-dimensional vertical flow in unsaturated homogenous soil:

Ψ-based form

$$C(\Psi)\frac{\partial \Psi}{\partial t}-\frac{\partial}{\partial z}\left[K(\Psi)\left(\frac{\partial \Psi}{\partial z}-1\right)\right]=0 \tag{1}$$

θ-based form

$$\frac{\partial \theta}{\partial t}-\frac{\partial}{\partial z}\left[D(\theta)\frac{\partial \theta}{\partial z}+K(\theta)\right]=0 \tag{2}$$

Mixed form

$$\frac{\partial \theta}{\partial t}-\frac{\partial}{\partial z}\left[K(\Psi)\left(\frac{\partial \Psi}{\partial z}-1\right)\right]=0 \tag{3}$$

where, z is the vertical coordinate taken positive downwards, t is time, Ψ is the pressure head, θ is the volumetric moisture content, K is the effective hydraulic conductivity, $C(\Psi)\equiv\partial\theta/\partial\Psi$ is the specific moisture capacity, and $D(\theta)\equiv K(\theta)/C(\theta)$ is the unsaturated diffusivity. In order to solve above equations, constitutive relationships between dependent variables Ψ and θ, and between nonlinear terms K and Ψ (or θ) have to be specified. In this study, the van Genuchten (1980) equations are used for these relationships.

θ - Ψ relationship

$$S_e=\frac{1}{\left[1+(\alpha|\Psi|)^n\right]^m} \tag{4}$$

where, α and n are soil property parameters with a relation of $m=1-1/n$, and S_e is the effective saturation defined as

$$S_e=\frac{\theta-\theta_r}{\theta_s-\theta_r} \tag{5}$$

where, θ_s and θ_r are saturated and residual moisture content of soils, respectively. Substituting Eq. (4) into Eq. (5) and rearranging the equation gives

$$\theta(\Psi)=(\theta_s-\theta_r)S_e+\theta_r=\frac{\theta_s-\theta_r}{\left[1+(\alpha|\Psi|)^n\right]^m}+\theta_r \tag{6}$$

K - θ relationship

$$K(\Psi)=K_sS_e^{1/2}\left[1-(1-S_e^{1/m})^m\right]^2=K_s\frac{\left\{1-(\alpha|\Psi|)^{n-1}\left[1+(\alpha|\Psi|)^n\right]^{-m}\right\}^2}{\left[1+(\alpha|\Psi|)^n\right]^{m/2}} \tag{7}$$

where, K_s is the saturated hydraulic conductivity.

2.2. Numerical Scheme

The Crank-Nicolson method was considered to solve nonlinear Richards equation. However, the fully implicit finite difference method is used in this study, since numerical solutions using the Crank-Nicolson scheme with explicit linearized values of C and K yield large global mass balance errors. The fully implicit finite difference formulation of the Ψ-based form at time level $n+1$ is written as

$$C_{i,n+1}^{m}D_t\Psi_{i,n+1}^{m+1}-\frac{1}{\Delta z}\left[K_{i-1/2,n+1}^{m}\left(\frac{\Psi_{i+1,n+1}^{m+1}-\Psi_{i,n+1}^{m+1}}{\Delta z}-1\right)-K_{i-1/2,n+1}^{m}\left(\frac{\Psi_{i,n+1}^{m+1}-\Psi_{i-1,n+1}^{m+1}}{\Delta z}-1\right)\right]=0 \tag{8}$$

where, i and n are the discretized space and time domain respectively;

$D_t\Psi_{i,n+1}^{m+1}\equiv(\Psi_{i,n+1}^{m+1}-\Psi_{i,n})/\Delta t$ is the backward Euler method operator, Δt is the time step, and Δz is a constant node spacing; m is the iteration level; $C_{i,n+1}^{m}$ and $K_{i\pm1/2,n+1}^{m}$ denote specific moisture and hydraulic conductivity evaluated using $\Psi_{i,n+1}^{m}$, respectively. Because C and K are nonlinear function of Ψ, Picard iteration method is used to obtain sequential estimation of the unknown $\Psi_{i,n+1}^{m+1}$ using the latest values of $C_{i,n+1}^{m}$ and $K_{i\pm1/2,n+1}^{m}$; the convergence of Picard iteration scheme was calculated by $\max\left|\frac{(\Psi^{m+1}-\Psi^{m})}{\Psi^{m+1}}\right|\le10^{-8}$; $K_{i\pm1/2,n+1}^{m}$ is the average effective hydraulic conductivity of the adjacent nodes i and $i\pm1$. The finite difference equation collecting each term of Eq. (8) is

$$\frac{1}{\Delta t}C_{i,n+1}^{m}\Psi_{i,n+1}^{m+1}-\frac{1}{\Delta z}\left[\frac{K_{i-1/2,n+1}^{m}}{\Delta z}\Psi_{i-1,n+1}^{m+1}-\left(\frac{K_{i-1/2,n+1}^{m}}{\Delta z}+\frac{K_{i+1/2,n+1}^{m}}{\Delta z}\right)\Psi_{i,n+1}^{m+1}+\frac{K_{i+1/2,n+1}^{m}}{\Delta z}\Psi_{i+1,n+1}^{m+1}\right]$$

$$= \frac{1}{\Delta t} C^m_{i,n+1} \Psi_{i,n} - \frac{1}{\Delta z}\left(K^m_{i+1/2,n+1} - K^m_{i-1/2,n+1}\right) \tag{9}$$

The finite difference approximation of the mixed formulation (Eq. (3)) is obtained by expanding the term $\theta^{m+1}_{i,n+1}$ in $D_t\theta^{m+1}_{i,n+1}$ with a truncated Taylor series about $\Psi^{m+1}_{i,n+1}$.

$$\theta^{m+1}_{i,n+1} \approx \theta^m_{i,n+1} + C^m_{i,n+1}\left(\Psi^{m+1}_{i,n+1} - \Psi^m_{i,n+1}\right) \tag{10}$$

Substituting Eq. (10) into the finite difference approximation of Eq. (3) and collecting terms gives

$$\frac{1}{\Delta t} C^m_{i,n+1}\Psi^{m+1}_{i,n+1} - \frac{1}{\Delta z}\left[\frac{K^m_{i-1/2,n+1}}{\Delta z}\Psi^{m+1}_{i-1,n+1} - \left(\frac{K^m_{i-1/2,n+1}}{\Delta z} + \frac{K^m_{i+1/2,n+1}}{\Delta z}\right)\Psi^{m+1}_{i,n+1} + \frac{K^m_{i+1/2,n+1}}{\Delta z}\Psi^{m+1}_{i+1,n+1}\right]$$
$$= \frac{1}{\Delta t} C^m_{i,n+1}\Psi^m_{i,n+1} - D_t\theta^m_{i,n+1} - \frac{1}{\Delta z}\left(K^m_{i+1/2,n+1} - K^m_{i-1/2,n+1}\right) \tag{11}$$

Comparing Eq. (11) with Eq. (9), we can find that two discretized formulations differ only by the right-hand side terms. The mixed formulation is independent of C at convergence, because $\frac{1}{\Delta t} C^m_{i,n+1}\Psi^m_{i,n+1} \approx 0$ at convergence.

2.3. Evaluation of K and C

Averaged effective hydraulic conductivity

The node-centered finite difference approximation requires the evaluation of the hydraulic conductivity at half nodal point, $i \pm 1/2$, as in general the parameter K is spatially referenced to the internodes. The internodal hydraulic conductivity $K^m_{i\pm 1/2}$ is here estimated using the geometric averaging scheme proposed and verified by Haverkamp et al. (1979), Schnabel et al. (1984), Romano et al. (1998), and Brunone et al. (2003):

$$K^m_{i\pm 1/2,n+1} = \sqrt{K^m_{i,n+1} \cdot K^m_{i\pm 1,n+1}} \tag{12}$$

Specific moisture capacity

Mass balance errors observed in the solution of Ψ-based form are associated with the expansion of the storage term (Celia et al., 1990).

$$\frac{\partial\theta}{\partial t} = \frac{\partial\theta}{\partial\Psi}\frac{\partial\Psi}{\partial t} = C\frac{\partial\Psi}{\partial t} \tag{13}$$

The evaluation of C with analytical derivatives of $\theta(\Psi)$ ie., $C(\Psi) \equiv \partial\theta/\partial\Psi$ (tangent approximation) can not be considered mass conservative because $\theta(\Psi)$ is nonlinear for most typical soils. For finite difference approximation a mass conservative form of C is developed from Eq. (13) which leads to the standard chord slope approximation of C

$$C^m_{i,n+1} = \frac{D_t\theta^m_{i,n+1}}{D_t\Psi^m_{i,n+1}} = \frac{\theta^m_{i,n+1} - \theta_{i,n}}{\Psi^m_{i,n+1} - \Psi_{i,n}} \tag{14}$$

And, Eq. (14) can be expanded as

$$\frac{1}{\Delta t} C^m_{i,n+1}\Psi^m_{i,n+1} = \frac{1}{\Delta t} C^m_{i,n+1}\Psi_{i,n} + D_t\theta^m_{i,n+1} \tag{15}$$

Substituting Eq. (15) into the right-hand side of Eq. (11) reveals that the finite difference formulation of Ψ-based form Eq. (9) and mixed form Eq. (11) are identical when the standard chord slope approximation of C is employed.

3. Model Validation and Selection

The Ψ-based form and mixed form of Richards equation were solved by the fully implicit finite difference method. The two model results were compared with a problem chosen from the literature (Celia et al., 1990) in order to validate the finite difference model developed in this study and to select a mass conservative numerical model for sensitivity analysis.

The test problem involves vertical moisture infiltration under constant surface ponding. The problem predicts infiltration of a homogeneous soil column of 1 m, which is initially dry. The soil parameters are $\alpha = 0.0335$ /cm, n = 2, m = 5, $\theta_s = 0.368$, and $\theta_r = 0.102$, $K_s = 0.00922$ cm/s. Initial and boundary conditions are Ψ(z,0) = -1000 cm, Ψ(0,t) = -75 cm, and Ψ(1m,t) = -1000 cm. The solutions correspond to the simulated solution at an elapsed time of 1 day. The result of test simulation using finite difference model developed in this study is exactly compatible with the finite difference solution of the problem chosen from the literature of Celia et al. (1990) including the fact that the solution using $\Delta t = 144$ sec did not converge in nonlinear iteration.

The numerical solution based on the mixed formulation shows a mass conservative property, while the result based on the Ψ-based formulation yields large mass balance errors.

4. Sensitivity Analysis

The parameter α is a measure of capillary fringe thickness, and n is the pore size distribution. Both two parameters have significant influence on moisture movement through the unsaturated zone. The sensitivity analysis was performed using the finite difference model of the mixed equation form with $\Delta z = 1.0$ cm and $\Delta t = 1.0$ sec. To study the sensitivity of infiltration, two kinds of sensitivity analyses were performed. The first method is that α and n are varied over a wide range to cover most of field soils, while keeping other properties of the soil which were used to validate and demonstrate the mass conservative numerical model. The second method is to estimate the infiltration in unsaturated zone for typical types of homogenous soils such as clay, loam, sand, and silt.

4.1. Sensitivity of α

A range from 0.01 /cm to 0.1 /cm is considered for the sensitivity of parameter α, which can cover most of field soils. Table 1 shows the values of other parameters n, K_s, θ_s, and θ_r fixed as constants.

Table 1. Soil properties for sensitivity of α

α	n	K_s	θ_s	θ_r
0.01, 0.0335, 0.05, 0.1	2	0.00992	0.368	0.102

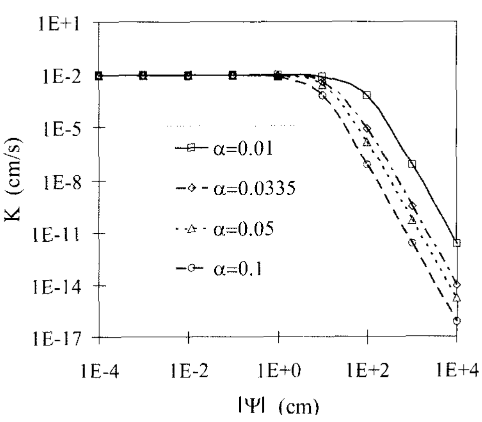

Fig. 1. Hydraulic conductivity-pressure head relation for α.

Fig. 1 denotes the relationship of K and Ψ for the values of α considered in this study. The hydraulic conductivity decreases as α increases. Fig. 2 shows that as the value of α increases, the wetting front moves at slower rates because the hydraulic conductivity decreases with increasing α. We can also find that the wetting front with a smaller α value has moved deeper than that with a larger α value for one-day simulation under the same initial pressure head.

4.2. Sensitivity of n

The sensitivity of parameter n is examined for a range

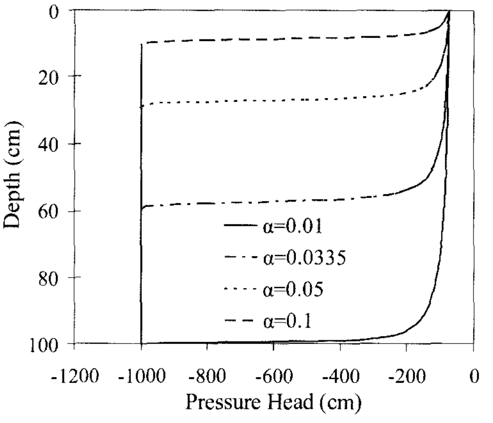

Fig. 2. Pressure head profiles for α at t=1 day.

Table 2. Soil properties for sensitivity of n

n	α	K_s	θ_s	θ_r
1.5, 2, 2.5, 3, 3,5	0.0335	0.00992	0.368	0.102

from 1.5 to 3.5 that can cover most of field soils. The other parameters α, K_s, θ_s, and θ_r are constants as shown in Table 2.

Fig. 3 shows the relationship of K and Ψ for the values of n considered in this study. As n increases, the hydraulic conductivity slightly increases for pressure heads less than the value at the point P in Fig. 3, and then beyond this point the hydraulic conductivity decreases with respect to n. Fig. 4 shows the depth of wetting front for different values of n after one-day simulation. As n increases, the wetting front depth becomes smaller because the hydraulic conductivity decreases with increasing n. Note that the values of pressure heads used in this study are beyond the point P. If pressure heads at the initial time and on the soil surface are less than the value at the point P in Fig. 3, the wetting front may move faster as the value of n increases. Therefore, the sensitivity of n on the infiltration process is complicated due to the various relationships between K and Ψ for different n values.

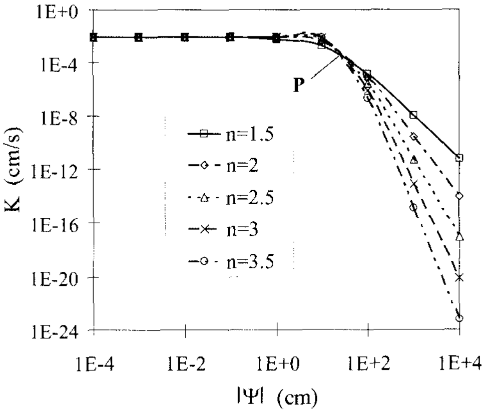

Fig. 3. Hydraulic conductivity-pressure head relation for n.

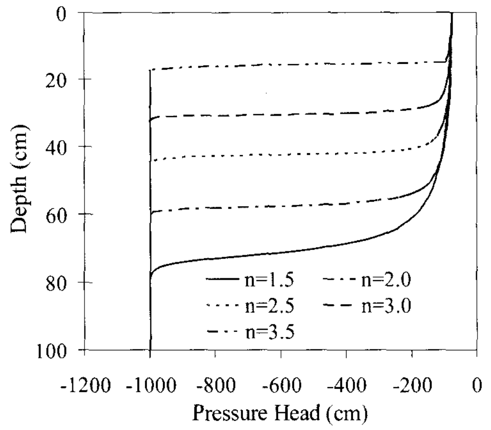

Fig. 4. Pressure head profiles for n at t=1 day.

4.3. Simulations for Different Soil Types

The finite difference model was applied to different types of soils. The same boundary conditions and initial conditions of the previous sensitivity analysis were used in this simulation. The soil properties for each soil type are shown in Table 3.

Fig. 5 denotes the pressure head profiles for different types of soils after 2, 4, and 6-hrs simulations. It is observed that the wetting front of silt moves fastest and the depth of wetting front of clay is smallest. The depth of wetting is sensitive to the value of α, and the silt soil has the smallest α value in the four typical soil types. The depth of wetting for the sand is similar to that of clay because the sand soil has the greatest value of K_s while it has larger values of α and n than those of clay.

Table 3. Class-average values of soil properties from van Genuchten (1980)

Type	θ_r	θ_s	α	n	K_s
Clay	0.098	0.495	0.015	1.25	1.71E-04
Loam	0.061	0.399	0.0111	1.47	1.40E-04
Sand	0.053	0.375	0.0352	3.18	7.44E-03
Silt	0.05	0.489	0.0066	1.68	5.06E-04

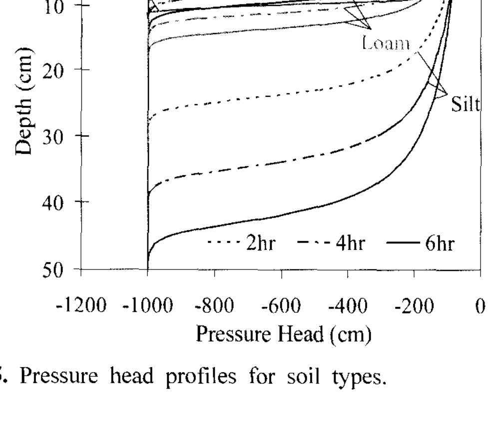

Fig. 5. Pressure head profiles for soil types.

5. Conclusion

A numerical flow model was developed for one-dimensional vertical flow in unsaturated soils using fully implicit finite difference method, and the model was validated by comparing the model results with a problem from the literature.

Sensitivity analysis of infiltration processes to variation in unsaturated soil parameters α and n was performed. As the value of α and n increases, the wetting front moves slower because unsaturated hydraulic conductivity decreases with respect to α and n. However, the effect of n on infiltration is complicated because the movement of wetting front depends on the initial pressure head and the head applied at the top. The wetting front of silt moves fastest and the depths of wetting front of clay and sand are small for given initial and boundary conditions. The depth of wetting is sensitive to the value of α and the silt soil has the smallest α value in the four typical soil types.

국문요약

질량보존의 법칙과 Darcy의 법칙으로 표현되는 Richards 방정식은 비포화대의 토양수분흐름을 모의하는데 널리 사용되어 왔다. Richards 방정식은 압력수두의 항으로 표현되는 방정식, 토양수분의 항으로 표현되는 방정식, 그리고 이 둘을 혼합한 형태의 방정식 등, 세가지 형태로 표현할 수 있다. 고차의 비선형 항들을 포함하는 이 편미분방정식들을 수치해석방법으로 풀 때, 질량 비보존을 수반하는 오류의 결과가 초래될 수 있다. 세가지 방정식들 중 혼합형 Richards 방정식이, 다른 추가적인 계산없이 질량을 온전히 보존하는 것으로 알려져 있다. 이 연구의 목적은 동질성 토양에서의 1차원적 연직방향 비포화수 흐름모의를 위해, Richards 방정식의 질량보존적 수치해석법을 완전음해 유한차분법으로 개발하고, 이를 통해 민감도 분석을 실시하여 토양특성인자들과 토양종류에 따른 침투율의 변화를 살펴보는 데 있다.

References

Allen, M. B. and Murphy, C., A Finite Element Collocation Method for Variably Saturated Flows in Porous Media, *Numer. Meth. Partial Diff. Eqn.*, **3**, pp. 229-239 (1985).

Brunone, B., Ferrante, M., Romano, N. and Santini, A., Numerical Simulations of One-Dimensional Infiltration into Layered Soils with the Richards Equation Using Different Estimates of the Interlayer Conductivity, *Vadose Zone J.*, **2**, pp. 193-200. (2003).

Celia, M. A., Ahuja, L. R. and Pinder, G. F., Orthogonal Collocation and Alternating Direction Procedures for Unsaturated Flow Problems, *Adv. Water Resour.*, **10**(4), 178-187 (1987).

Celia, M. A., Bouloutons, E. T. and Zarba, R. L., A General Mass-conservative Numerical Solution for the Unsaturated Flow Equation, *Water Resour. Res.*, **26**(7), pp. 1483-1496 (1990).

Freeze, R. A., Three-dimensional, Transient, Saturated-unsaturated Flow in a Groundwater Basin, *Water Resour. Res.*, **7**(2), pp. 347-366 (1971).

Haverkamp, R., Vaclin, M., Touma, J., Wierenga, P. J. and Vachaud, G., A Comparison of Numerical Simulation Models for One-dimensional Infiltration, *Soil Sci. Soc. Am. J.*, **41**, pp. 285-294 (1977).

Haverkamp, R. and Vauclin, M., A Note on Estimating Finite Difference Interblock Hydraulic Conductivity Values for Transient Unsaturated Flow Problems, *Water Resour. Res.*, **15**, pp. 181-187 (1979).

Hayhoe, H. N., Study of the Relative Efficiency of Finite Difference and Galerkin Techniques for Modeling Soil-water Transfer, *Water Resour. Res.*, **14**(1), pp. 97-102 (1978).

Huyakorn, P. S., Thomas, S. D. and Thompson, B. M., Techniques for Making Finite Elements Competitive in Modeling Flow in Variably Saturated Porous Media, *Water Resour. Res.*, **20**(8), pp. 1099-1115 (1984).

Milly, P. C. D., A mass-conservative procedure for time-stepping in models of unsaturated flow, *Adv. Water Resour.*, **8**, pp. 32-36 (1985).

Narasimhan, T. N. and Witherspoon, P. A., An Integrated Finite Difference Method for Analyzing Fluid Flow in Porous Media, *Water Resour. Res.*, **12**, pp. 57-64 (1976).

Neumann, S. P., Saturated-unsaturated Seepage by Finite Elements, *J. Hyd. Div., ASCE*, **HY12**, pp. 2233-2250 (1973).

Richards, L., Capillary conduction of liquids through porous mediums, *Physics*, **1**, pp. 318-333 (1931)

Romano, N., Brunone, B. and Santini, A., Numerical Analysis of One-dimensional Unsaturated Flow in layered soils, *Adv. Water Resour.*, **21**, pp. 315-324 (1998).

Schnabel, R. R., and Richie, E. B., Calculation of Internodal Conductances for Unsaturated Flow Simulations: A comparison, *Soil Sci. Soc. Am. J.*, **48**, pp. 1006-1010 (1984).

van Genuchten, M. T., A Closed-form Equation for Predicting the Hydraulic Conductivity of Unsaturated Soils, *Soil Sci. Soc. Am. J.*, **44**(5), pp. 982-898 (1980).