



Transition Between Constitutive Equations and the Mechanics of Water Flow in Unsaturated Soil: Numerical Simulations

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ARTICLE INFO

ABSTRACT

Article history:

Received 4 September 2020

Received in revised form 30 October 2020

Accepted 31 October 2020

Available online 11 January 2021

Richards' partial differential equation normally governs water flows in soil. It can be utilized to investigate water infiltration in the soil. A case study of the Haverkamp's water infiltration simulation into Yolo Light Clay was carried out. A common practice to change between the hydraulic functions (from Haverkamp to van Genuchten) could cause a discrepancy in the simulation results. Hence, the first objective is to modify van Genuchten's equations to reproduce the water infiltration result that was obtained using the Haverkamp constitutive functions. The method used was able to recreate water infiltration by increasing the fitting parameters of the van Genuchten constitutive functions. The second objective is to identify the mechanism governing the flow of water. The soil water diffusivity and the hydraulic conductivity were responsible for the flux of water in the soil. The Richards' equation was discretized using a finite difference method, and the algebraic solution was coded into Simply Fortran 2008.

Keywords:

Water flow in soil; unsaturated soil;
water flux; water adsorption

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1. Introduction

Richards' equation consists of a governing equation that is used to describe the water flow in subsurface porous media such as soil in unsaturated conditions [1]. It is continuously subjected to numerical investigation [2–11]. The modeling of water distribution using the equation has essential applications in climate science, agriculture and also ecosystem management [12]. Among many applications, Zeide [13] has reported the use of Richards' equation in the tree growth modelling prediction. Soil scientists, agronomists, and irrigation engineers have found the equation useful to relate to plant water uptake, and fertilizers and pesticides advection and dispersion in the soils [14]. In addition, other equation like Navier-Stokes could be used to investigate flow in porous media, but the flow investigation would be more complicated [15,16].

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A nonlinear partial differential equation represents the governing equation. It is often difficult to approximate because it does not have a closed-form analytical solution [17]. Richards' equation consists of two parts; the water flux expression that is similar to Darcy's law, and the continuity equation is used to monitor the mass balance of water flux in and out of a control volume. The equation to describe the unsaturated flow can be written in three forms, as follows

$$\text{Head-based, } C(\psi_m) \frac{\partial \psi_m}{\partial t} = \frac{\partial}{\partial z} \left(K \frac{\partial \psi_m}{\partial z} \right) - \frac{\partial K}{\partial z} \quad (1)$$

$$\text{Mixed-based, } \frac{\partial \theta_L}{\partial t} = \frac{\partial}{\partial z} \left(K \frac{\partial \psi_m}{\partial z} \right) - \frac{\partial K}{\partial z} \quad (2)$$

$$\text{Saturation-based, } \frac{\partial \theta_L}{\partial t} = \frac{\partial}{\partial z} \left(D(\theta_L) \frac{\partial \theta_L}{\partial z} \right) - \frac{\partial K}{\partial z} \quad (3)$$

where the detailed description on Eq. (1) was described in Rathfelder and Abriola [18]. Similarly, Kavetski *et al.*, [19] and Zeng and Decker [20] have provided a detailed explanation for mixed- and saturation-based of Richards' equation. To implement the equation, the soil water retention relation (θ_L as a function of ψ_m) and the unsaturated hydraulic conductivity relation (K as a function of ψ_m) must be known from measurement [21].

Water infiltration is one of the common applications for Richards' equation, and the water infiltrated medium is normally assumed as homogeneous and isotropic [22]. In reality, the water flux regime could be affected depending on the locations in the soil that could be resulted from different transport coefficients such as the soil water retention curve and hydraulic conductivity relations, including, a spatial variation of different saturated volumetric water contents [23]. There are different constitutive functions to describe the water retention curve and hydraulic conductivity relation, for example, van Genuchten [24], Campbell [25], and Haverkamp *et al.*, [26]. The experimental dataset described by a constitutive function used in Richards' equation will affect the water infiltration profile.

Different water infiltration profiles resulting from different constitutive functions are a well-known problem, but there are still no published records on a solution. This problem is commonplace when one is applying published coefficients of a particular water retention curve equation, for example, Haverkamp [26], to conduct simulation study, and then, attempt to change between constitutive function equations, for example, from Haverkamp *et al.*, [26] to van Genuchten [24] equation. One would have to recreate the dataset using Haverkamp equation coefficients first and then, redo the curve-fitting on the dataset using the Genuchten equation, hence, resulting in different water infiltration profiles. Therefore, the first objective of the study is to provide a solution for the transition between constitutive equations and be able to produce similar water infiltration profile.

Richards' equation, as described by Hopmans [21], is a mass conservation equation and includes the expression of Darcy's law. An in-depth description of Richards' equation is also given by Germann [27] from the perspective of the Navier-Stokes equation. However, taking the case of water infiltration as an example, the influence of the coefficients ($D(\psi_m)$, K , $\theta_L - \psi_m$) as in Eq. (3) on water infiltration profile have not been discussed prior. The second objective of this study is to reveal the mechanics behind Richards' equation as governed by the coefficients.

2. Methodology

Richards' equation was reported as not behaving as mass conserving equation when using Eq. (1) [28]. Eq. (2) and (3) were free from the mass conservation problem. The water-based Richards' equation in Eq. (3) was chosen and used in this study because the volumetric water content appeared in the independent and dependent variables which would ease the programming effort. The $D(\psi_m)$ is the soil water diffusivity ($\text{m}^2 \cdot \text{s}^{-1}$), and it is given by

$$D(\psi_m) = K(\psi_m) \frac{\partial \psi_m}{\partial \theta_L} \quad (4)$$

where $\frac{\partial \psi_m}{\partial \theta_L}$ is the derivative of matric suction (ψ_m , -m) with respect to volumetric water content (θ_L , $\text{m}^3 \cdot \text{m}^{-3}$), and $K(\psi_m)$ is the hydraulic conductivity ($\text{m} \cdot \text{s}^{-1}$) of the soil.

The constitutive functions from Haverkamp *et al.*, [26] for the water retention curve ($\theta_L - \psi_m$) and hydraulic conductivity ($K(\psi_m)$) are given by

$$\psi_m = -10^{-2} \exp \left[\frac{\alpha(\theta_s - \theta_r)}{\theta_L - \theta_r} - \alpha \right]^{1/\beta} \quad (5)$$

$$K = K_s \frac{A}{A + \left(\exp \left[\frac{\alpha(\theta_s - \theta_r)}{\theta_L - \theta_r} - \alpha \right]^{1/\beta} \right)^B} \quad (6)$$

van Genuchten's [24] water retention curve and hydraulic functions are given below

$$\psi_m = -\frac{1}{\alpha_1} \left[\left(\frac{\theta_s - \theta_r}{\theta_L - \theta_r} \right)^{1/m} - 1 \right]^{1/n} \quad (7)$$

$$K = K_s \left(\frac{\theta_L - \theta_r}{\theta_s - \theta_r} \right)^L \left\{ 1 - \left[1 - \left(\frac{\theta_L - \theta_r}{\theta_s - \theta_r} \right)^{1/m} \right]^m \right\}^2 \quad (8)$$

where α , α_1 , A , B , β , L and n are fitting parameters, θ_s is saturated water content ($\text{m}^3 \cdot \text{m}^{-3}$), θ_r is residual water content ($\text{m}^3 \cdot \text{m}^{-3}$), K_s is saturated hydraulic conductivity ($\text{m} \cdot \text{s}^{-1}$), and m is also fitting parameter where $m = 1 - 1/n$.

In order to implement Richards' equation, Eq. (3) was discretized into algebraic equations using the cell-centered finite-difference method, as follows,

$$\frac{\theta_{L(k)}^{n+1} - \theta_{L(k)}^n}{\Delta t} = \frac{K_{k+1/2} (\partial \psi_m / \partial \theta_L)_{k+1/2}}{(\Delta z)^2} (\theta_{L(k+1)}^{n+1} - \theta_{L(k)}^{n+1}) - \frac{K_{k-1/2} (\partial \psi_m / \partial \theta_L)_{k-1/2}}{(\Delta z)^2} (\theta_{L(k)}^{n+1} - \theta_{L(k-1)}^{n+1}) - \frac{K_{k+1/2} \vec{k} - K_{k-1/2} \vec{k}}{\Delta z} \quad (9)$$

where k indicates a centre cell in the z -direction of a cartesian coordinate system, $+1/2$ refers to the interface of cell located between the cell k and $k+1$, $-1/2$ refers to cell interface between the cells $k-1$ and k , n indicates the current time, $n+1$ indicates new time, and Δ refers to the difference of a parameter. Eq. (9) is oriented positive downward, as does Eq. (3). A complete description of the numerical scheme was explained in Goh and Noborio [29]. The equations were coded in Fortran.

Water infiltration phenomenon was used as a case study. The soil type used was Yolo light clay. A schematic diagram as in Figure 1 provides a simplistic view of the model environment.

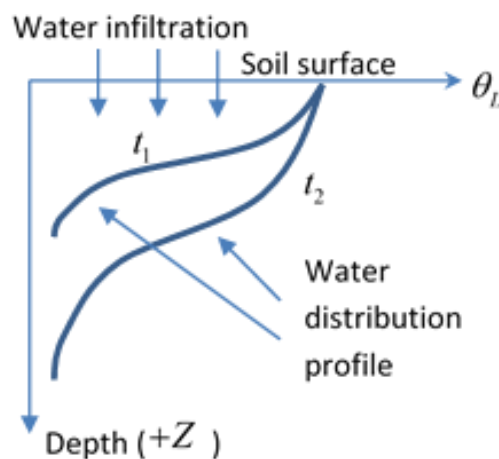


Fig. 1. Water distribution in the soil by a schematic diagram for soil water infiltration profile

3. Results

3.1 Validation of Simulation Results with Philip's Semianalytical Solution

The Yolo light clay soil was initially wet with a homogeneous soil moisture content of $0.2376 \text{ m}^3 \cdot \text{m}^{-3}$. The clay properties are shown in Table 1. The water infiltration begins with the upper soil body saturated with $0.495 \text{ m}^3 \cdot \text{m}^{-3}$ soil moisture content, and the lower soil body was assumed permeable to water, that is to say, water is free to move in and out. The total soil depth was taken as 2.5 m. The soil depth was further divided into 100 cells, where each cell represents 2.5 cm. Each cell was governed by Eq. (9), and the cells were simulated simultaneously in Fortran.

To make sure Richards' equation was programmed correctly, the simulation has to be validated either by experimentation or an analytical solution dataset. In this case study, we used Philip's semianalytical solution [30–32] to validate the Fortran code. The results are shown in Figure 2. The

R-squared showed a good match between Fortran simulation and the analytical solution of water infiltration profiles at 1.16, 11.6 and 34.7 days that were 0.9992, 0.9988 and 0.9994, respectively.

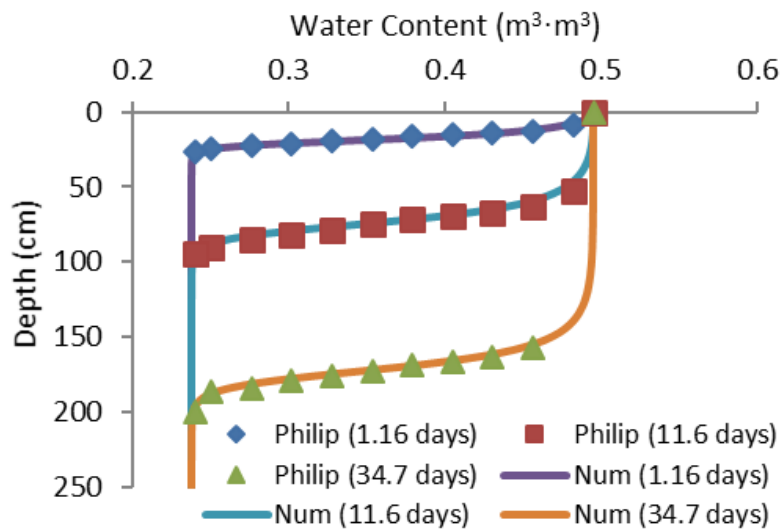


Fig. 2. Water distribution in the soil by water infiltration profile in Yolo light clay after 1.16, 11.6 and 34.7 days. Philip and Num referred to Philip’s semianalytical solution and the Fortran coded numerical simulation, respectively

Table 1

The soil type is Yolo light clay. The parameters used were retrieved from Haverkamp *et al.*, [26]

Parameters						
α	θ_r ($m^3 \cdot m^{-3}$)	θ_s ($m^3 \cdot m^{-3}$)	β	A	B	K_s ($m \cdot s^{-1}$)
739	0.124	0.495	4	124.6	1.77	1.23×10^{-7}

Note: α , A , B and β are fitting parameters, θ_s is saturated water content, θ_r is residual water content, and K_s is saturated hydraulic conductivity

3.2 The Problem of Transition Between Constitutive Equations

Water retention curve is also known as a water characteristic curve. There are many water characteristic curve equation [33], and a new equation is continuously being proposed [34]. Hence, it would be impossible to address all the transition issues between all the equations. However, a simple case study would be discussed here as an example to demonstrate the technique used, which can be referred to as a transition method in solving similar problems.

Changing the characteristic curve equation, for example from Haverkamp to van Genuchten equations, with the same dataset could result in different water infiltration profile, as shown in Figure 4(a). This is because fitting Haverkamp’s and van Genuchten’s equations on the same dataset produced different curves for the relationship between soil water content and soil matric suction, and also resulted in the different curves between the hydraulic conductivity and water saturation. Figure 3(a) shows the modified van Genuchten (R-squared = 0.899) is closer to the soil water content data than the original version of van Genuchten (R-squared = 0.894). Similarly, in Figure 3(b), the modified van Genuchten (R-squared = 0.999) resulted in better hydraulic conductivity that is closely approximate the data than the unmodified van Genuchten (R-squared = 0.919).

As shown in Figure 4(a), at 34.7 days, the original van Genuchten equation simulation had under predicted the water infiltration profile. In achieving objective one that is to have equal water infiltration profiles that transition from Haverkamp's to van Genuchten's equations, the classical van Genuchten - Mualem formulas in Eq. (7) and (8) were modified. Their modification that is modified van Genuchten, with appropriate parameters m_1 , n_1 , m_2 , and n_2 , in Eq. (10) and (11).

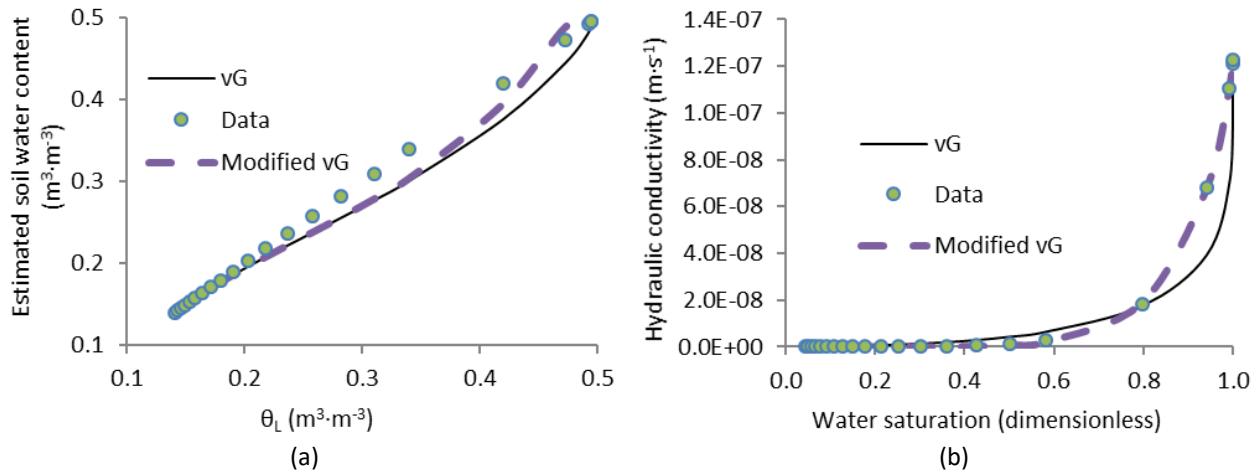


Fig. 3. The curve-fitted results of modified van Genuchten (as Modified vG), original van Genuchten (as vG) and data for (a) soil water content, and (b) hydraulic conductivity

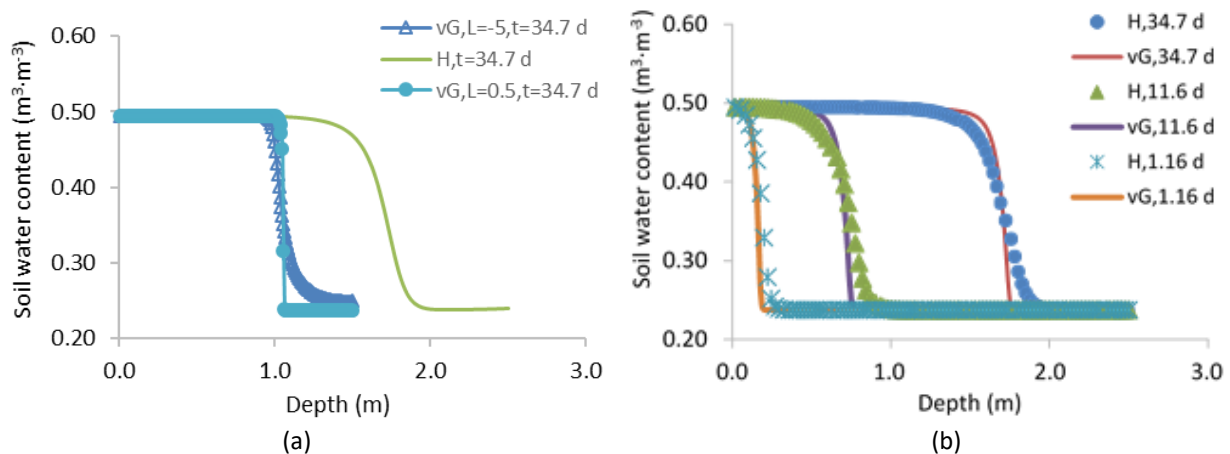


Fig. 4. Water infiltration profile for Genuchten's and Haverkamp's equations simulated at: (a) 34.7 days with m , n , α_1 curve-fitted, while L fixed at 0.5 or -5 for original van Genuchten; and (b) 1.16, 11.6, 34.7 days with L , m_1 , n_1 , m_2 , n_2 , α_1 curve-fitted for modified van Genuchten. Note: vG and H corresponding to Genuchten and Haverkamp

$$\psi_m = -\frac{1}{\alpha_1} \left[\left(\frac{\theta_s - \theta_r}{\theta_L - \theta_r} \right)^{1/m_1} - 1 \right]^{1/n_1} \tag{10}$$

$$K = K_s \left(\frac{\theta_L - \theta_r}{\theta_s - \theta_r} \right)^L \left\{ 1 - \left[1 - \left(\frac{\theta_L - \theta_r}{\theta_s - \theta_r} \right)^{1/n_2} \right]^{m_2} \right\}^2 \tag{11}$$

The curve-fitting parameters were increased from 3 to 6. The intention of the modification was to increase the ability of the Eq. (10) and (11) to have a better curve-fitting ability than Eq. (7) and (8). Figure 4(b) has proven the effectiveness of this method which was able to recreate the centre of the water infiltration front, possible beyond 34.7 days.

Therefore, the best practice is to make the equation parameters unbound between the characteristic curve equation (Eq. (10)) and the hydraulic conductivity equation (Eq. (11)). This practice can be applied to other studies without much difficulty.

3.3 The Mechanics of Richards' Equation

Figure 4(b) showed that Richards' equation, using the improved Genuchten Eq. (10) and (11) has significantly improved the simulation to match with those of Haverkamp. The water infiltration front appeared sharply from 34.7 to 1.16 days of simulation. Although the improved Genuchten's equation is able to reproduce the water-front centre, it reproduces a sharper water front than that of Haverkamp's. The Genuchten water-front appeared to increase in the high water content spatial region sharply and sharply decreased at the low water content spatial region. This occurrence can be explained by the relationship between hydraulic conductivity (K) and soil moisture content, as in Figure 5(a), where the Genuchten curve gives a higher hydraulic conductivity at the high water content region and a lower hydraulic conductivity at the low water content region. Figure 5(b) shows the rarely reported relation between $\frac{\partial \psi_m}{\partial \theta_L}$ and the soil moisture content. The graph shows a concave curve with a minimum which reached at $0.4586 \text{ m}^3 \cdot \text{m}^{-3}$, which indicates a minimum gradient. Knowing that $D(\theta_L)$ in Eq. (4) consist of $K(\theta_L)$ and $\frac{\partial \psi_m}{\partial \theta_L}$, the former variable is always high at high soil moisture content as in Figure 5(a), whereas the latter variable would have to depend on the region soil wetness. This means that $(\frac{\partial \psi_m}{\partial \theta_L})_{k-1/2} - (\frac{\partial \psi_m}{\partial \theta_L})_{k+1/2}$ in space may not always be positive in value because it depends on the level of soil wetness. Whereas the $D(\theta_L)_{k-1/2} - D(\theta_L)_{k+1/2}$ is always positive for water infiltration front as long as the water is continuously infiltrating into the soil, which explains the increasing soil water content with time in the soil depth.

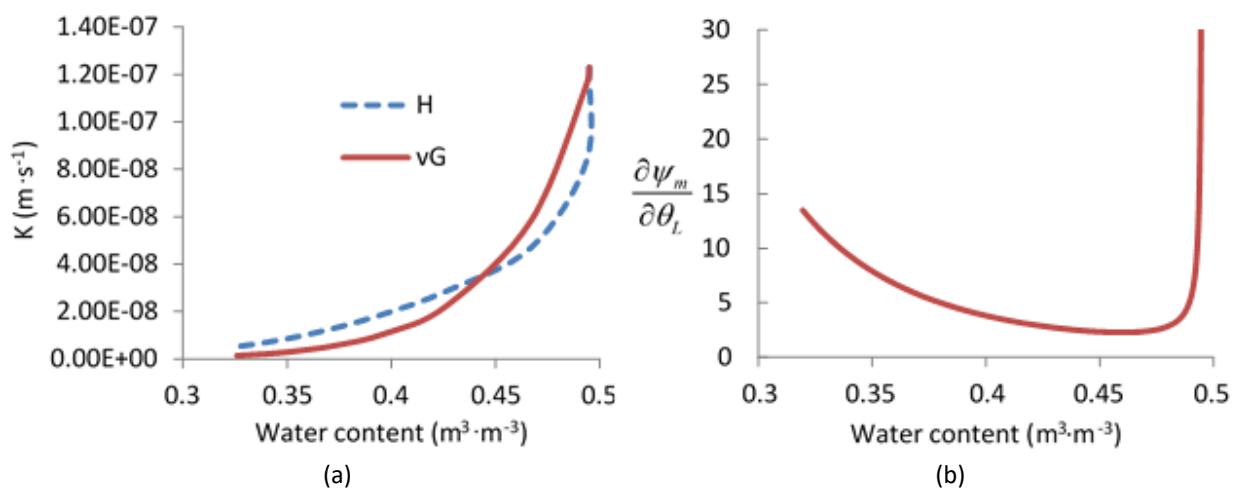


Fig. 5. (a) Hydraulic conductivity varies with soil moisture content, and (b) the derivative of soil matric suction with respect to moisture content varies with soil moisture content

4. Conclusions

Richards' equation is important to govern water flow in the unsaturated soil, which acts as an interface between the atmosphere and the groundwater. Richards' equation which is frequently used in conjunction with other constitutive equations (water characteristic curve and hydraulic functions), does not allow easy transition between equations, for example from Haverkamp's to Genuchten's. In the first objective, we have demonstrated that a simple modification of the existing Genuchten variables was able to reproduce the water infiltration front. In the second objective, we have discussed the importance of understanding the variables in Richards' equation in order to be able to understand the mechanics of water transport and also to be able to describe the observed sharp water infiltration front produced from using Genuchten's equation. The hidden property of the derivative of soil matric suction, with respect to the soil moisture content, is often overlooked but it has influenced the influx of water into the soil.

Acknowledgement

This research was supported by Ministry of Higher Education (MOHE) through Fundamental Research Grants Scheme FRGS/1/2020/STG08/UMT/02/2.

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