

6-2017

The Soil Moisture Velocity Equation

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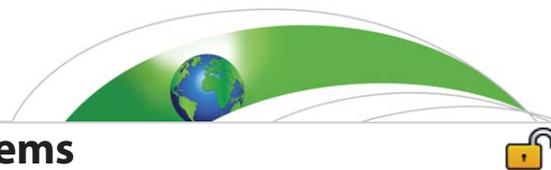
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RESEARCH ARTICLE

The soil moisture velocity equation

10.1002/2017MS000931

Key Points:

- We have converted the one-dimensional Richards partial differential equation into a new form that is much easier to solve
- Our new equation is an ordinary differential equation that is accurate, reliable, guaranteed to converge and to conserve mass
- Neglecting the diffusion term in our new equation has a negligible effect on the calculated flux of water, with errors less than 1%

Supporting Information:

- Supporting Information S1

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Citation:

Ogden, F. L., M. B. Allen, W. Lai, J. Zhu, M. Seo, C. C. Douglas, and C. A. Talbot (2017), The soil moisture velocity equation, *J. Adv. Model. Earth Syst.*, 9, doi:10.1002/2017MS000931.

Received 27 JAN 2017

Accepted 19 MAY 2017

Accepted article online 23 MAY 2017

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Abstract Numerical solution of the one-dimensional Richards' equation is the recommended method for coupling groundwater to the atmosphere through the vadose zone in hyperresolution Earth system models, but requires fine spatial discretization, is computationally expensive, and may not converge due to mathematical degeneracy or when sharp wetting fronts occur. We transformed the one-dimensional Richards' equation into a new equation that describes the velocity of moisture content values in an unsaturated soil under the actions of capillarity and gravity. We call this new equation the Soil Moisture Velocity Equation (SMVE). The SMVE consists of two terms: an advection-like term that accounts for gravity and the integrated capillary drive of the wetting front, and a diffusion-like term that describes the flux due to the shape of the wetting front capillarity profile divided by the vertical gradient of the capillary pressure head. The SMVE advection-like term can be converted to a relatively easy to solve ordinary differential equation (ODE) using the method of lines and solved using a finite moisture-content discretization. Comparing against analytical solutions of Richards' equation shows that the SMVE advection-like term is >99% accurate for calculating infiltration fluxes neglecting the diffusion-like term. The ODE solution of the SMVE advection-like term is accurate, computationally efficient and reliable for calculating one-dimensional vadose zone fluxes in Earth system and large-scale coupled models of land-atmosphere interaction. It is also well suited for use in inverse problems such as when repeat remote sensing observations are used to infer soil hydraulic properties or soil moisture.

Plain Language Summary Since its original publication in 1922, the so-called Richards' equation has been the only rigorous way to couple groundwater to the land surface through the unsaturated zone that lies between the water table and land surface. The soil moisture distribution and properties of the soil in the unsaturated zone determine how much precipitation becomes runoff or infiltrates into the soil. During non-rainy periods, the soil moisture distribution determines how much water is available for use by plants or for groundwater recharge. Richards' equation is arguably the most difficult equation to accurately and reliably solve in hydrologic science. The first somewhat robust computational solution was not published until 1990. We have converted Richards' equation into a new form that is much simpler to solve and 99% accurate for calculating the vertical flow of water in unsaturated soil in response to rainfall and changes in groundwater levels. Where Richards' equation allows calculation of the change in degree of saturation with time at a point in an unsaturated soil, our simpler equation allows calculation of the speed of travel of specific moisture contents in the soil. For this reason we call this new equation the Soil Moisture Velocity Equation (SMVE).

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1. Introduction

Earth system models are used to simulate interactions between the atmosphere, ocean, land surface, and sub-surface. On the land surface, these models calculate hydrological fluxes using numerical schemes of various levels of detail and sophistication. Earth system models are undergoing active development [Döll and Fiedler, 2008; Peters-Lidard et al., 2007; Van Beek et al., 2011; Gosling and Arnell, 2011; Hurrell et al., 2013] and the representation of hydrological processes in these models varies [Clark et al., 2015]. Presently, Earth system models

generally run at coarse spatial resolutions such as minutes of longitude [Koster et al., 2010], while there is a recognition that increased resolution is desirable and represents a “grand challenge” [Wood et al., 2011; Beven and Cloke, 2012; Wood et al., 2012] and that increased resolution will allow or require improved process level descriptions, which are at present considered rudimentary in some respects [Clark et al., 2015].

Up to now, the only way to accurately calculate fluxes of water in the unsaturated or vadose zone has been the equation attributed to Richards [1931], which was earlier posited by Richardson [1922]. Richards’ equation can be written with water content θ or capillary head ψ as the dependent variable. The one-dimensional Richards’ equation in “mixed water content form” because it contains both the water content θ and the capillary head $\psi(\theta)$ is

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z} \left[K(\theta) \left(\frac{\partial \psi(\theta)}{\partial z} - 1 \right) \right], \quad (1)$$

where z is the vertical coordinate (positive downward) [L], t is time [T], $\theta = \theta(z,t)$ is the volumetric soil moisture content, $\psi(\theta)$ is the empirical soil hydraulic capillary head function [L], and $K(\theta)$ is the empirical unsaturated hydraulic conductivity function [L T⁻¹].

One of the major difficulties affecting the numerical solution of Richards equation is the extreme nonlinearity of the empirical $K(\theta)$ and $\psi(\theta)$ functions, which together are often called “water constitutive relations” for a particular soil. Richards’ [1931] equation is arguably the most difficult equation to solve in all of hydrological science, as discussed at some length later.

In wetter climates the depth from the land surface to the groundwater table is the dominant variable affecting the partitioning of precipitation and energy at the Earth surface. Figure 1a shows an idealized hillslope in a humid or semihumid environment. Notice that the water table is near the land surface, soils are deep and well developed, trees are widespread, and groundwater fed streamflow is perennial. In this setting the groundwater table can rise to the land surface and produce saturation-excess runoff, which can cause the numerical solution of Richards’ equation to become degenerate as the capillary head in the soil nears zero at saturation. During extended dry periods there can be an upward flux of water from the water table into the soil profile, where that water is used by plants. This upward flux of soil water is counter-intuitive, and one of the reasons why two-way vadose zone coupling is needed in Earth system models.

In arid and semiarid regions the situation is as shown in Figure 1b, the groundwater table is typically far from the land surface, and soil moisture is generally the dominant variable controlling the partitioning of moisture and heat fluxes. Runoff only occurs during rainfall at the hillslope scale, when sharp wetting fronts develop during infiltration into dry soils. Sharp wetting fronts can cause difficulty with numerical solutions of Richards’ equation because the spatial gradients of the terms in the Richards equation become difficult to evaluate accurately especially with a fixed spatial discretization.

Both Figures 1a and 1b show what are essentially commonplace situations that occur at the hyperresolution modeling scale. Many land-surface and Earth system models simulate these situations using a quasi-3-D

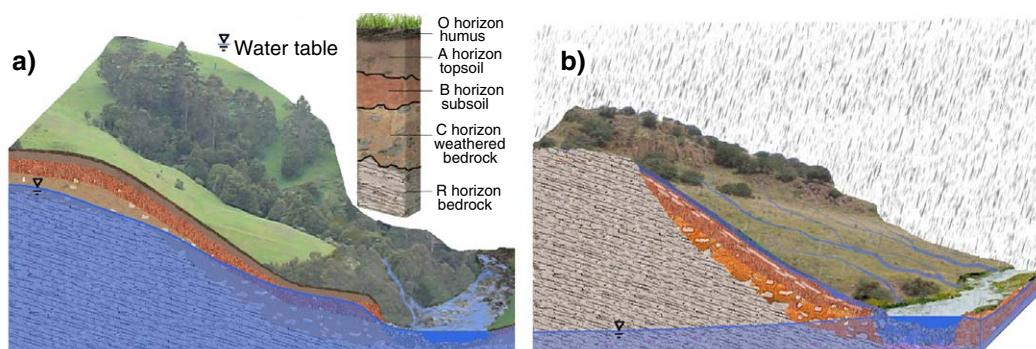


Figure 1. Groundwater table configurations at the 100 m hillslope scale for (a) humid/semihumid and (b) semiarid/arid environments. Inset shows example soil profile.

approach, with hyperresolution (sub 100 m) two-dimensional overland and groundwater routing schemes coupled with a one-dimensional vadose zone solution. At horizontal scales greater than approximately 10 m, lateral fluxes in the unsaturated zone may be neglected at the timescale of hydrological events [Or *et al.*, 2015].

Earth systems models must simulate the coupling between the atmosphere and subsurface so that the influence of groundwater is reflected in the simulation, and important hydrological fluxes are accurately simulated [Larsen *et al.*, 2016; Maxwell and Condon, 2016]. Among the most important of these fluxes are the exchange of water between the land and atmosphere, precipitation partitioning by the soil, evapotranspiration, movement of water in the vadose zone, groundwater recharge, and the upward flux of water from the groundwater table to the vadose zone [Good *et al.*, 2015].

Present Earth system models contain a wide variety of soil moisture dynamical formulations, ranging from numerical solutions of Richards' [1931] equation to a variety of empirical approaches [Clark *et al.*, 2015]. Furthermore, Earth system models contain a variety of approximations and assumptions regarding runoff generation, soil moisture uptake by plants, groundwater flow routing, and surface flow routing. Some Earth system models do not consider two-way fluxes between the root zone and groundwater [Clark *et al.*, 2015]. Clark *et al.* [2015] recommended the use of Richards' equation to couple the groundwater-soil-plant-atmosphere continuum in Earth system models to avoid conceptualizations of vadose zone fluxes.

Up to now, the numerical solution of Richards' equation is the only rigorous technique to solve vadose zone water fluxes [Vereecken *et al.*, 2016]. Richards' equation is a nonlinear, degenerate, parabolic-elliptic partial differential equation (PDE). The elliptic nature of the solution can arise when capillary head is the primary variable, which is common in simulations of layered soils because capillary head is the continuous variable while water content is discontinuous across layers [List and Radu, 2016]. Numerical solvers for parabolic PDEs are not appropriate for elliptic PDEs.

The Richards equation is called a "degenerate" PDE because the strongly nonlinear coefficients in the equation approach zero in parts of the solution domain. For instance, the soil capillary pressure approaches zero as the soil approaches saturation and the unsaturated hydraulic conductivity approaches zero as the soil dries. This latter property leads to the existence of wetting fronts in which moisture content values propagate with finite speed, in contrast to the behavior of solutions to linear analogs such as the heat equation [Barenblatt, 1952; Swartzendruber, 1969; Aronson, 1986; Vasquez, 2007]. Furthermore, the properties of the PDE change from parabolic to elliptic as the soil becomes saturated. Nonlinearities and the degeneracy make the design and analysis of numerical schemes to solve Richards' equation very difficult [Celia *et al.*, 1990; Arbogast *et al.*, 1996; Lott *et al.*, 2012; List and Radu, 2016]. Hydrologically, nearly saturated soils are extremely important because it is in this state where runoff is produced, and it is exactly near saturation that Richards' equation can become computationally most expensive and unreliable [Paniconi *et al.*, 2003].

While the derivation of Richards' equation is simple, designing a computational solution methodology that is efficient, reliable, and mass conservative is difficult [List and Radu, 2016]. Numerical solutions of Richards' equation have been developed in one, two, and three spatial dimensions. Discretization of the solution domain into spatial coordinates imposes a spatial resolution on the solution that interacts with the time step and convergence criteria to produce a solution. The accuracy of this solution depends strongly on the space-time discretization, boundary conditions, dimensionality, linearizations, and convergence criteria [Celia *et al.*, 1990; Arbogast *et al.*, 1996; Miller *et al.*, 1998; Pop *et al.*, 1999; Van Dam and Feddes, 2000; Kavetski *et al.*, 2002; Lott *et al.*, 2012; Lai *et al.*, 2015; List and Radu, 2016]. The spatial resolution of the Richards' equation solution domain must be fine enough to provide representative bulk properties of the medium and to accurately represent the effects of calculated fluxes on the change in moisture content. The spatial discretization must be comparable to the size of the "representative elementary volume" or REV, associated with continuum-scale modeling of the porous medium. The REV requirement for infiltration excess runoff that is common in arid and semiarid areas, or in some watersheds with deep, fine-textured soils was examined by Downer and Ogden [2004], in the case of the one-dimensional (vertical) solution of Richards' equation. Downer and Ogden [2004] found that if the vertical discretization near the land surface was more than about 1 cm, then the REV assumption was violated, and the soil moisture did not respond properly to applied rainfall. In essence, when the discretization was larger than the appropriate REV scale, water did not infiltrate the soil properly during rainfall, and as a result the soil remained less conductive to water than with finer

vertical discretizations. *Downer and Ogden* [2004] found that “effective” parameters could be used to overcome this effect, but these changes in the parameter values resulted in too much infiltration as the soil surface approached saturation. Two and three-dimensional Richards’ equation simulations of even small catchments at appropriate spatial resolutions require very long run times [*Ameli et al.*, 2015], when the solution domain is required to meet the REV assumption.

The two and three-dimensional numerical solution of Richards’ equation is therefore unsuited to earth system models and large-scale models of land-atmosphere interaction because of REV assumption requirements and the computational difficulties associated with strong nonlinearities and degeneracy, not to mention the limited lateral scales of unsaturated zone flow [*Or et al.*, 2015].

In general, the utility of a Richards’ equation solution is affected by the degree of linearization employed in the solution, as well as the selection of space/time discretization and convergence criteria [*Twarakavi et al.*, 2009]. For example, robustness can be improved by reducing the spatial resolution of the solution domain, decreasing the required convergence criteria or both. The negative consequences of such actions are to increase mass balance errors, or violate the representative area volume assumption by using low solution resolution, which requires “effective” parameter values of questionable utility, or both.

In the *Richards* [1931] equation, the water content or head is the dependent variable. In this paper we convert the *Richards* [1931] equation into a form where the dependent variable is the velocity of particular moisture content, and we call this new equation the Soil Moisture Velocity Equation (SMVE). The authors believe that the change in dependent variable justifies a change in equation name. The SMVE is equivalent to Richards’ equation but a major difference is that the SMVE consists of separate advection-like and diffusion-like flux terms. *Kowalczyk et al.* [2006] developed an approximate splitting method to separate the diffusive and gravity term in *Richards*’ [1931] equation. This is quite different from our approach, which actually reformulates Richards’ equation into a form where the flux due to the shape of the capillary wetting front is a completely separate term that may be ignored.

Following *Talbot and Ogden* [2008], who derived an advective solution by extending the *Green and Ampt* [1911] approach to the infiltration problem in a finite moisture-content solution domain, *Ogden et al.* [2015a] derived the advection-like term of the SMVE using unsaturated zone conservation of mass and Darcy-Buckingham unsaturated flow theory and used the method of lines (MOL) to convert the advection-like term into an ordinary differential equation. *Ogden et al.* [2015a] compared the Finite Moisture Content (FMC) solution of the SMVE advection-like term against the one-dimensional numerical solution of Richards’ equation using the HYDRUS one-dimensional solver [*Simunek et al.*, 1996]. This test involved simulation of 8 months of rainfall on a loam soil with a shallow water table fixed at 1 m below the land surface. Out of 263 cm of total rainfall, the difference in cumulative infiltration between the FMC solution of the SMVE advection-like term and HYDRUS-1D was only 0.7 cm, an error of only 0.3%. The results shown by *Ogden et al.* [2015a] led to the discovery of the full SMVE reported in this paper.

All numerical solutions of the Richards equation introduce uncertainties due to unique issues related to numerical approximations, algorithmic approximations such as linearization, convergence criteria, and the strong nonlinearities of the soil water constitutive relations. The development of numerical solutions of the Richards equation is an area of active research [*List and Radu*, 2016]. To avoid comparison against numerical solutions of Richards’ equation is to avoid questions regarding the appropriate selection of spatial discretization, time step, and other details associated with a particular Richards’ equation solver.

In this study we evaluated the effect of neglecting the SMVE diffusion-like term by comparing the FMC solution of the SMVE advection-like term against two analytical solutions of Richards’ equation identified by *Ross and Parlange* [1994]. Comparison against analytical solutions of the Richards equation is an excellent way to test solution methods, because it avoids complications associated with the numerical solution of *Richards*’ equation. It also allows evaluation of the effect of neglecting the diffusion term of the SMVE on the actual shape of the wetting front profiles. Finally, this comparison allows us to evaluate the performance of the FMC solution of the SMVE for predicting fluxes. Our hypothesis is that neglecting the diffusion-like flux term in the SMVE will not have an appreciable effect on the fluxes calculated using the advection-like term of the SMVE, because the diffusion-like flux term should have a mean near zero.

2. Derivation of the Soil Moisture Velocity Equation

We derive the SMVE starting with the one-dimensional *Richards'* equation (equation (1)) in mixed form that includes both the water content with the capillary head constitutive relationship.

By the chain rule of differentiation,

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z} K(\theta(z, t)) \frac{\partial}{\partial z} \psi(\theta(z, t)) + K(\theta) \frac{\partial^2}{\partial z^2} \psi(\theta(z, t)) - \frac{\partial}{\partial z} K(\theta(z, t)). \quad (2)$$

Assuming that the soil constitutive relations for unsaturated hydraulic conductivity and capillarity are solely functions of moisture content, $K=K(\theta)$ and $\psi=\psi(\theta)$, respectively, we have

$$\frac{\partial \theta}{\partial t} = K'(\theta) \psi'(\theta) \left(\frac{\partial \theta}{\partial z} \right)^2 + K(\theta) \left[\psi''(\theta) \left(\frac{\partial \theta}{\partial z} \right)^2 + \psi'(\theta) \frac{\partial^2 \theta}{\partial z^2} \right] - K'(\theta) \frac{\partial \theta}{\partial z}. \quad (3)$$

At least locally, this equation implicitly defines a function $z=Z_R(\theta, t)$ giving the vertical location of a specified value of moisture content θ at time t . By the implicit function theorem, $\frac{\partial Z_R(\theta, t)}{\partial t} = -\frac{\partial \theta / \partial t}{\partial \theta / \partial z}$ and dividing both sides of equation (3) by $-\partial \theta / \partial z$ yields

$$\frac{\partial Z_R}{\partial t} = -K'(\theta) \psi'(\theta) \frac{\partial \theta}{\partial z} - K(\theta) \psi''(\theta) \frac{\partial \theta}{\partial z} - K(\theta) \psi'(\theta) \frac{\partial^2 \theta / \partial z^2}{\partial \theta / \partial z} + K'(\theta), \quad (4)$$

which can be written as

$$\frac{\partial Z_R}{\partial t} = -K'(\theta) \left[\frac{\partial \psi(\theta)}{\partial z} - 1 \right] - K(\theta) \left[\psi''(\theta) \frac{\partial \theta}{\partial z} + \psi'(\theta) \frac{\partial^2 \theta / \partial z^2}{\partial \theta / \partial z} \right]. \quad (5)$$

Equation (5) can be simplified to

$$\frac{\partial Z_R}{\partial t} = -K'(\theta) \left[\frac{\partial \psi(\theta)}{\partial z} - 1 \right] - D(\theta) \frac{\partial^2 \psi / \partial z^2}{\partial \psi / \partial z}, \quad (6)$$

where $D(\theta) = K(\theta) \partial \psi / \partial \theta$ is the soil water diffusivity. Because velocity is the dependent variable in equation (6), we call it the Soil Moisture Velocity Equation (SMVE).

The first term on the right-hand side of the SMVE (equation (6)), which we refer to as the advection-like term, was derived by *Ogden et al.* [2015a]. The second term on the right-hand side of equation (6), which we call the diffusion-like term, is the diffusive flux due to the shape of the soil water capillarity profile divided by the vertical gradient of the soil water capillarity. This diffusion-like term has several interesting properties. The soil water diffusivity $D(\theta)$ is not constant so the mean diffusive flux in the numerator of this term does not have to be equal to 0, but may be small so as to not significantly affect the mean flux

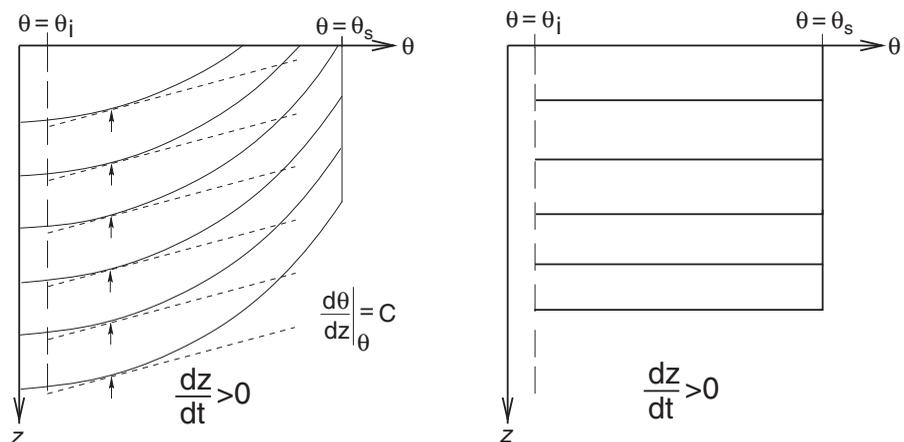


Figure 2. Conditions where the diffusion-like flux term in equation (6) will be zero. In this figure θ_s represents the saturated water content, while θ_i represents the initial water content.

calculated using the SMVE when neglecting this term [Zhu *et al.*, 2016]. In the case of a sharp wetting front, which is common in the case of infiltration into dry fine-textured soils, the denominator $\partial\psi/\partial z$ can become large in magnitude and cause this term to vanish. With reference to Figure 2, if the soil water capillarity ψ is not a function of z , or if $\partial\psi/\partial z$ is a constant in time, then the numerator of the diffusion-like term will equal zero. As a result, both of these cases represent conditions where numerical solvers of the one-dimensional Richards equation have difficulties converging [Ross, 1990; Tocci *et al.*, 1997].

3. Finite Moisture Content Solution Method

Following Ogden *et al.* [2015a], we use the method of lines to approximate the partial derivatives in the first advection-like term on the right-hand side of equation (6), and we neglect the second diffusion-like term. The solution is obtained using a one-dimensional finite moisture-content discretization shown in Figure 3a, which shows the pore space of a soil divided uniformly into regions of moisture content $\Delta\theta$, which we refer to as “bins.” It is important to note that θ is not a spatial dimension; it is the value of the moisture content at a particular depth in the soil z . The only spatial dimension in our discretization is the vertical dimension, z , defined as positive downward. There is no fractional water content within a bin. They are binary in that at a particular depth z , a bin is either filled or empty. Talbot and Ogden [2008] showed that to the number of bins required to accurately simulate infiltration fluxes in a deep well-drained soil depends on the soil texture, and varies from 75 for clays to almost 400 for sands.

Defining θ_d as the moisture content of the right-most bin in the domain containing water, and θ_i as the soil moisture profile initial moisture content, with a ponded depth $h_p \geq 0$, the resulting advection-like term of the Soil Moisture Velocity Equation for the water content associated with the j th bin (Figure 3) is [Ogden *et al.*, 2015a]

$$\frac{dZ_j}{dt} = \frac{K(\theta_d) - K(\theta_i)}{\theta_d - \theta_i} \left[1 + \frac{\max(|\psi(\theta_d)|, G_{eff}) + h_p}{Z_j} \right]. \quad (7)$$

Following Talbot and Ogden [2008], we used a forward-Euler explicit finite volume solution, which requires a time step on the order of seconds during infiltration. We also take the wetting front effective capillary drive as the greater of the absolute value of the capillarity of the right-most bin containing water $\psi(\theta_d)$ or the effective minimum capillary drive of the wetting front G_{eff} [Morel-Seytoux *et al.*, 1996, equations (13) or (15)]. The finite moisture content (FMC) solution methodology does not require calculation of any spatial derivatives, which is a significant advantage over the classical Richards equation solution. This requires that the soil be uniform in layers, which is a common assumption. Soil layers may communicate through a head boundary condition in the FMC solution [Ogden *et al.*, 2015a]. We use equation (7) to calculate the advance of water in each bin. Because $K(\theta)$ is monotonically increasing, water to the right of the profile in θ -space will move faster than water on the left, particularly when the depth to the wetting front Z_j is considerably smaller in the right-most bins. When the distance to wetting fronts on the right of the finite water-content domain exceeds that on the left as shown in Figure 3a, it necessitates a step called “capillary relaxation” by Ogden *et al.* [2015a], after Moebius *et al.* [2012]. This process moves water from regions of low to high capillary head at the same elevation, in a free-energy minimization process that involves no change in potential energy, as shown in Figure 3b. Numerically, capillary relaxation is equivalent to a numerical sort that rank-orders the depth to the wetting front from maximum to minimum from left to right, but does not result in any net vertical motion of water.

Because the depth to the wetting front Z_j appears in the numerator of equation (7), when water advances into bin “ j ” that contains no water, $Z_j = 0$ resulting in a singularity. Following Talbot and Ogden [2008], we limit the

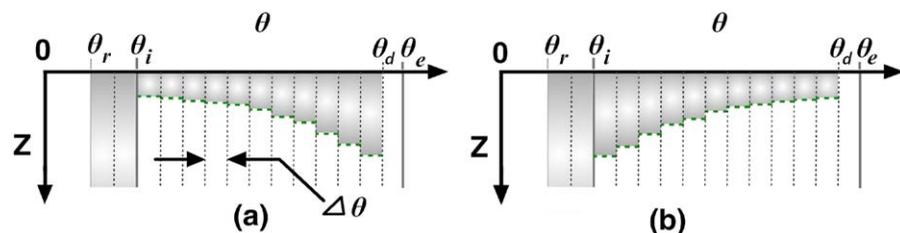


Figure 3. Finite moisture content solution domain, (a) after infiltration calculated using equation (7), (b) after capillary relaxation.

advance in bins without water to the maximum amount calculated by implicit solution of the *Green and Ampt* [1911] cumulative infiltration equation for time step Δt and discretization $\Delta\theta$. This initial advance depth is calculated once at the beginning of the simulation for each bin and saved for future use because it is a bin property.

4. Properties of Analytical Solutions Used in Comparison

In this section we describe two exact solutions of *Richards'* equation published by *Ross and Parlange* [1994] that were used to evaluate the performance of the SMVE advection-like term. These solutions are unique in that they assume soil water retention and unsaturated hydraulic conductivity functions that are artificial in that they are unlikely to represent a real soil. Their mathematical forms do, however, allow an exact solution of *Richards'* equation, and embody the monotonic properties of widely used soil water constitutive relations such as those by *Brooks and Corey* [1964] or *Mualem-Van Genuchten* [*Schaap and Leij*, 2000]. In this regard, they are plausible constitutive relations.

4.1. Power Law Soil Water Retention and Unsaturated Hydraulic Conductivity Functions

In terms of constitutive relations, the FMC solution of the SMVE can use any monotonic $K(\theta)$ and $\psi(\theta)$ functions, while the numerical solution of *Richards'* equation might require special treatment of soil constitutive relations for numerical stability and mass conservation [*Vogel and Cislserova*, 1988; *Vogel et al.*, 2001]. Here we define the relative saturation S_e as

$$S_e = \frac{\theta - \theta_r}{\theta_e - \theta_r}, \quad (8)$$

where θ is the volumetric soil moisture content [L^3L^{-3}], θ_e is the soil moisture content at effective saturation [L^3L^{-3}], and θ_r is the residual soil moisture content [L^3L^{-3}]. *Ross and Parlange* [1994] used the following power law functions of S_e to describe the soil water diffusivity D and unsaturated hydraulic conductivity K :

$$D(S_e) = D_1 S_e^n, \quad K(S_e) = K_1 S_e^{n+1}, \quad (9)$$

where D_1 and K_1 are constants, $(dK/d\theta)/D$ is a constant as suggested by *Gardner* [1958], and the dependence of D on θ is the same as *Brooks and Corey* [1964]. In equation (9), K is the unsaturated conductivity [LT^{-1}], D is the soil water diffusivity [L^2T^{-1}], S_e is the relative saturation, and K_1 , D_1 , and n are constant parameters. The soil water constitutive relations given in equation (9) result in the following water retention relationship, with h defined as the capillary head (negative for water under tension):

$$S_e = \exp\left(\frac{K_1 h}{D_1}\right), \text{ for } h < 0. \quad (10)$$

When the capillary head $h \geq 0$, the soil is saturated and the relative saturation $S_e = 1.0$.

For infiltration into a soil with uniform initial moisture content ($S_e(z, t = 0) = 0$), with water supplied at the surface ($z = 0$) at a rate $q = AS_e \theta_s$, the analytical solution can be derived [*Ross and Parlange*, 1994], but the solution depends on the value of the constant A . If $A < K_1$, the solution is

$$S_e(z, t) = \left[\frac{A}{K_1} \left(1 - \exp\left(\frac{-nK_1(At-z)}{D_1}\right) \right) \right]^{1/n}. \quad (11)$$

If $A > K_1$, ponding occurs at time t_p given by

$$t_p = \frac{D_1}{nK_1 A} \ln \frac{A}{A - K_1}. \quad (12)$$

Equation (11) is valid before ponding. After ponding, the profile is saturated for $z \leq A(t - t_p)$. For larger depths, equation (11) is still valid.

Note that in *Ross and Parlange* [1994], the surface flux $q = AS_e$ is used. In fact, it should be $q = AS_e \theta_s$, because after saturation, the saturated profile is moving at a rate $dz/dt = d(A(t - t_p))/dt = A$, considering the porosity θ_s , the water supply should be $A \theta_s$. The actual condition for ponding is $A \theta_s > K_1$. Because dimensionless variables are used throughout *Ross and Parlange* [1994], it is consistent. However, numerical simulation requires θ_r near 0.0 and θ_s near 1.0.

The use of t_p as ponding time by *Ross and Parlange* [1994] is a little misleading, since all water supplied to the surface is infiltrated and ponding never actually occurs, t_p would more accurately be called the time when the soil surface reaches a fully saturated state. After surface saturation, the moisture content profile moves downward with constant velocity $dz/dt = A$, which means there is no diffusion effect using the power law constitutive relations with this boundary condition. Also from equation (12), to find the position of leading front of $S_e = 0$, then $z_{\max} = At$, which means the leading front always moves at velocity equal to the parameter A , independent from the soil properties.

4.2. Nonlinear Soil Water Constitutive Relations

Ross and Parlange [1994] also proposed and tested nonlinear soil water constitutive relations with constants α , β , and γ ,

$$D(S_e) = \frac{\beta S_e}{(1 - \alpha S_e)^2}, \quad K(S_e) = \frac{\beta S_e}{(1 - \alpha S_e) \alpha \gamma}, \quad (13)$$

where the following relationship is satisfied:

$$K_1 = K(S_e = 1) = \frac{\beta}{(1 - \alpha) \alpha \gamma}, \quad (14)$$

which implies the following soil water retention curve:

$$S_e = \begin{cases} \frac{1}{\alpha} \left[1 - (1 - \alpha) \exp\left(\frac{-h}{\gamma}\right) \right] & h < 0 \\ 1 & h \geq 0 \end{cases} \quad (15)$$

For a rate of water input $A < K_1$ equation (13) in *Ross and Parlange* [1994] gives following:

$$S_e(z, t) = \frac{1}{\alpha} \left[1 + \frac{(1 - \alpha) K_1}{A - (1 - \alpha) K_1} \frac{1}{\exp[-(At - z)/\gamma] - A/[A - (1 - \alpha) K_1]} \right]. \quad (16)$$

Similar to the power law case, if the rate of water input $A > K_1$, then ponding occurs at time,

$$t_p = \frac{\gamma}{A} \ln \frac{A - (1 - \alpha) K_1}{A - K_1}, \quad A > K_1 \quad (17)$$

Equation (16) is valid before ponding. After ponding, the profile is saturated for $z \leq A(t - t_p)$, and at larger depths, equation (16) remains valid.

5. Results of Comparison

The following two sections describe the results of our comparison of the ODE SMVE advection-like term solved using the FMC method against both analytical solutions of Richards' equation by *Ross and Parlange* [1994]. This comparison evaluated the effects of neglecting the diffusion-like term in the SMVE, both in terms of the shape of the wetting front profiles at different times, and in terms of the cumulative infiltration.

5.1. Power Law Soil Water Retention and Unsaturated Hydraulic Conductivity Functions

We compared the analytical solution for ($A > K_1$) with SMVE-FMC simulation results for a power law soil characteristic curve. Parameters from *Ross and Parlange* [1994] were used: $A = 2.0 \text{ cm h}^{-1}$, $K_1 = 1.0 \text{ cm h}^{-1}$, $D_1 = 100 \text{ cm}^2 \text{ h}^{-1}$, and $n = (3, 4, 5, 6, 7, 8, 9)$ representing different soil types. $\theta_r = 0.001$ and $\theta_s = 1.0$ are used for all cases. Larger values of the exponent n (e.g., $n = 9$) produce more realistic looking soil water retention curves. The requirement by in equation (9) that the exponent on the unsaturated hydraulic conductivity be equal to $n + 1$ prevents the terms in equation (9) from matching real soils. This does not invalidate the solution, however.

The simulated moisture content profiles shown in Figure 4 were compared with analytical solutions at different times $t = 0.5t_p, t_p, t_{end}$, where t_{end} is time before surface runoff occurs in the finite moisture content simulation ($t_{end} = 16, 12, 9.8, 8.2, 7, 6.2, 5.6 \text{ h}$ for $n = 3.0$ to 9.0).

The simulation results from the power law soil water constitutive relations were analyzed in terms of cumulative infiltration. Those results are presented in Table 1.

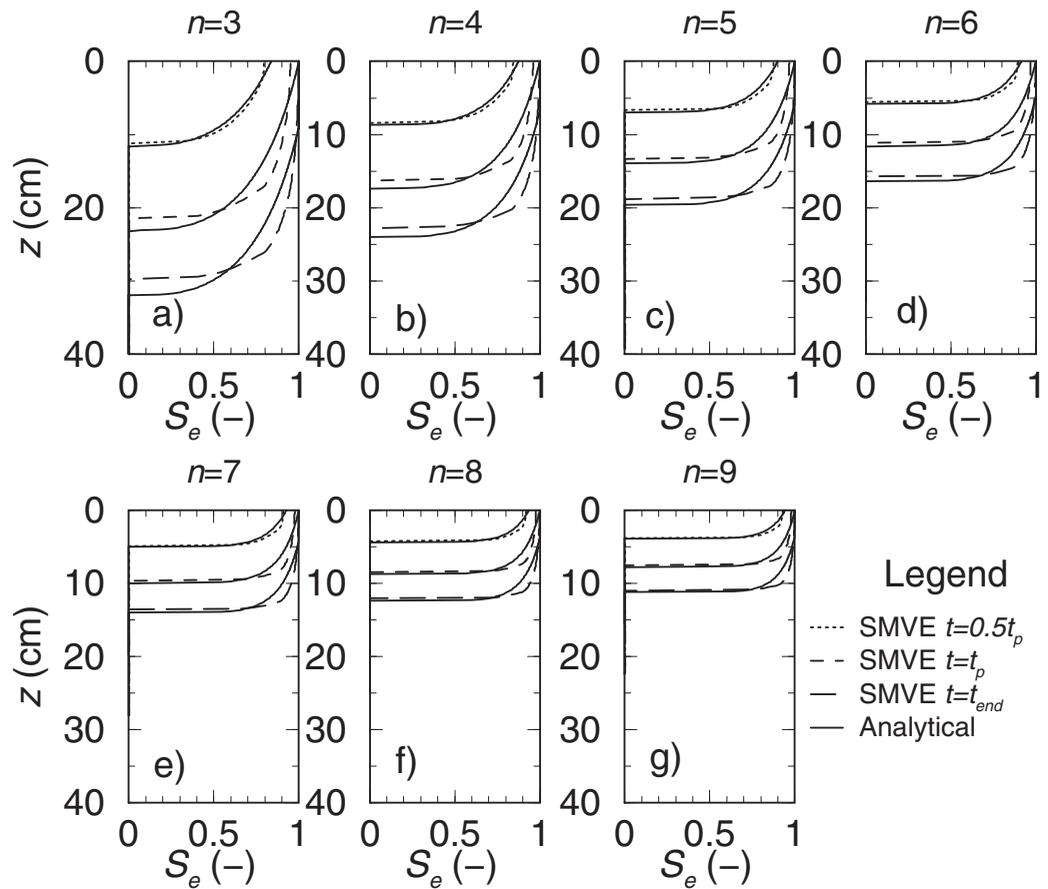


Figure 4. Results of tests with power law soil water constitutive relations.

Based on visual comparison of the wetting front profiles shown in Figure 3, the SMVE advection-like term seems to do a reasonably good job at matching the shape of the profiles. We used three different statistical measures to quantify the ability of the model to match the profiles, the Nash-Sutcliffe efficiency (NSE), the percent bias (PBIAS), and the root mean square error (RMSE).

The first measure, the Nash-Sutcliffe efficiency (NSE), compares the root mean squared error of the modeled prediction to the root means squared error when using the mean as a model. The NSE was calculated using the following equation:

$$NSE = 1 - \frac{\sum_{i=1}^N (\hat{z}_i - z_{ai})^2}{\sum_{i=1}^N (\mu_z - z_{ai})^2}, \quad (18)$$

where \hat{z}_i is the depth to the wetting front in the i th finite moisture content bin, z_{ai} is the depth to the wetting front at the moisture content corresponding to the i th finite moisture content bin by the analytical solution, μ_z is the mean of depth of the analytical solution, and N is the number of finite moisture content solution bins.

The NSE will be 1.0 with a perfect model, 0.0 if the model performs identically to the mean of the series, and negative if the model is not outperform the mean. Of course, the flatter the analytical solution,

Table 1. Errors of Cumulative Infiltration Predictions for Power Law Soil Water Constitutive Relations

| n | $t = 0.5t_p$ | $t = t_p$ | $t = t_{end}$ |
|-----|--------------|-----------|---------------|
| 3 | -0.04% | -0.23% | -0.09% |
| 4 | -0.02% | -0.30% | 0.15% |
| 5 | -0.87% | 0.23% | 0.20% |
| 6 | -0.60% | 0.07% | -0.18% |
| 7 | 0.63% | 0.23% | 0.17% |
| 8 | -0.88% | 0.04% | -0.09% |
| 9 | 0.33% | -0.41% | 0.43% |

Table 2. Statistical Measures of Simulated Wetting Front Shape in Power Law Test, for Different Values of the Power Law Soil Water Constitutive Relation Exponent n

| n | NSE | | | PBIAS (%) | | | RMSE (cm) | | |
|-----|--------------|-----------|---------------|--------------|-----------|---------------|--------------|-----------|---------------|
| | $t = 0.5t_p$ | $t = t_p$ | $t = t_{end}$ | $t = 0.5t_p$ | $t = t_p$ | $t = t_{end}$ | $t = 0.5t_p$ | $t = t_p$ | $t = t_{end}$ |
| 3 | 0.96 | 0.77 | 0.73 | -6.03 | -13.21 | -10.03 | 0.52 | 2.60 | 3.50 |
| 4 | 0.92 | 0.71 | 0.69 | -9.63 | -15.52 | -12.60 | 0.59 | 2.14 | 2.73 |
| 5 | 0.87 | 0.66 | 0.63 | -12.42 | -16.53 | -11.30 | 0.62 | 1.85 | 2.50 |
| 6 | 0.82 | 0.63 | 0.60 | -14.71 | -18.03 | -11.73 | 0.60 | 1.59 | 2.16 |
| 7 | 0.77 | 0.61 | 0.58 | -17.59 | -17.91 | -13.20 | 0.58 | 1.41 | 1.86 |
| 8 | 0.73 | 0.57 | 0.56 | -18.42 | -18.97 | -11.43 | 0.56 | 1.27 | 1.75 |
| 9 | 0.70 | 0.57 | 0.61 | -20.54 | -19.06 | -9.21 | 0.52 | 1.14 | 1.58 |

the more effective the mean will be at predicting the shape of the wetting front, and the model NSE might decrease.

The other statistical measures used to evaluate the solutions were the Root Mean Square Error (RMSE) and the Percent Bias (PBIAS). The RMSE was calculated using

$$RMSE = \sqrt{\frac{\sum_{i=1}^N (\hat{z}_i - z_{ai})^2}{N}}, \tag{19}$$

and the PBIAS was calculated using

$$PBIAS = \frac{\sum_{i=1}^N (z_{ai} - \hat{z}_i)}{\sum_{i=1}^N z_{ai}} * 100\%. \tag{20}$$

The results of the statistical comparison of the wetting front profile shapes are listed in Table 2.

The results of the statistical analysis of the wetting front profile shape given in Table 2 reveal that in terms of the NSE, the SMVE advection-like term performed reasonably well with $NSE > 0.55$ in all cases. The model performed better on soils with smaller exponent n , which would represent soils that are more like sands. The NSE values tended to decrease over time, largely because the profiles become flatter over time and are therefore better represented by the mean of the series. The NSE values did, however, remain significantly greater than 0, which indicated that the model outperformed the mean as a predictor for all times analyzed. In terms of PBIAS, the values of this statistic were negative and tended to decrease with time for soils with a larger exponent n , which would correspond to finer textured soils, but in general there was an increase of PBIAS seen with increasing n . The negative PBIAS indicates that on average, the wetting front depth is over-predicted. The net effect however, in terms of cumulative infiltration is very small as the results in Table 1 show. Similar to the NSE, the RMSE increased with time, and decreased with increasing exponent n .

5.2. Test of Nonlinear Soil Water Constitutive Relations

The analytical solutions ($A > K_1$) are compared with SMVE-FMC simulation results for the nonlinear soil characteristic curve proposed by Ross and Parlange [1994]. The parameters from Ross and Parlange [1994] were used in the comparison: $A = 2.0$ cm/h, $K_1 = 1.0$ cm/h, and $\gamma = 25$ cm. The parameter α is valid between 0 and 1, so results with α ranging from 0.1 to 0.95 are presented here. $\theta_r = 0.001$ and $\theta_s = 1.0$ were used for all tests. Larger values of the parameter α result in soil water constitutive relations that more closely resemble those for real soils.

The simulated moisture content profiles shown in Figure 5 were compared with analytical solutions at different times $t = 0.5t_p, t_p, t_{end}$, where t_{end} is time before surface runoff occurs in SMVE-FMC simulation ($t_{end} = 1.4, 2.7, 4, 5.2, 6.4, 7.5, 8.6, 9.7, 11.7$ h for $\alpha = 0.1$ to 0.8 and 0.95). Exact analytical and SMVE-FMC advection-like term solutions are plotted together at coincident times in Figure 5.

The cumulative infiltration in the case of the nonlinear soil water constitutive relations compared to the finite water-content solution of the SMVE advection-like term are listed in Table 3.

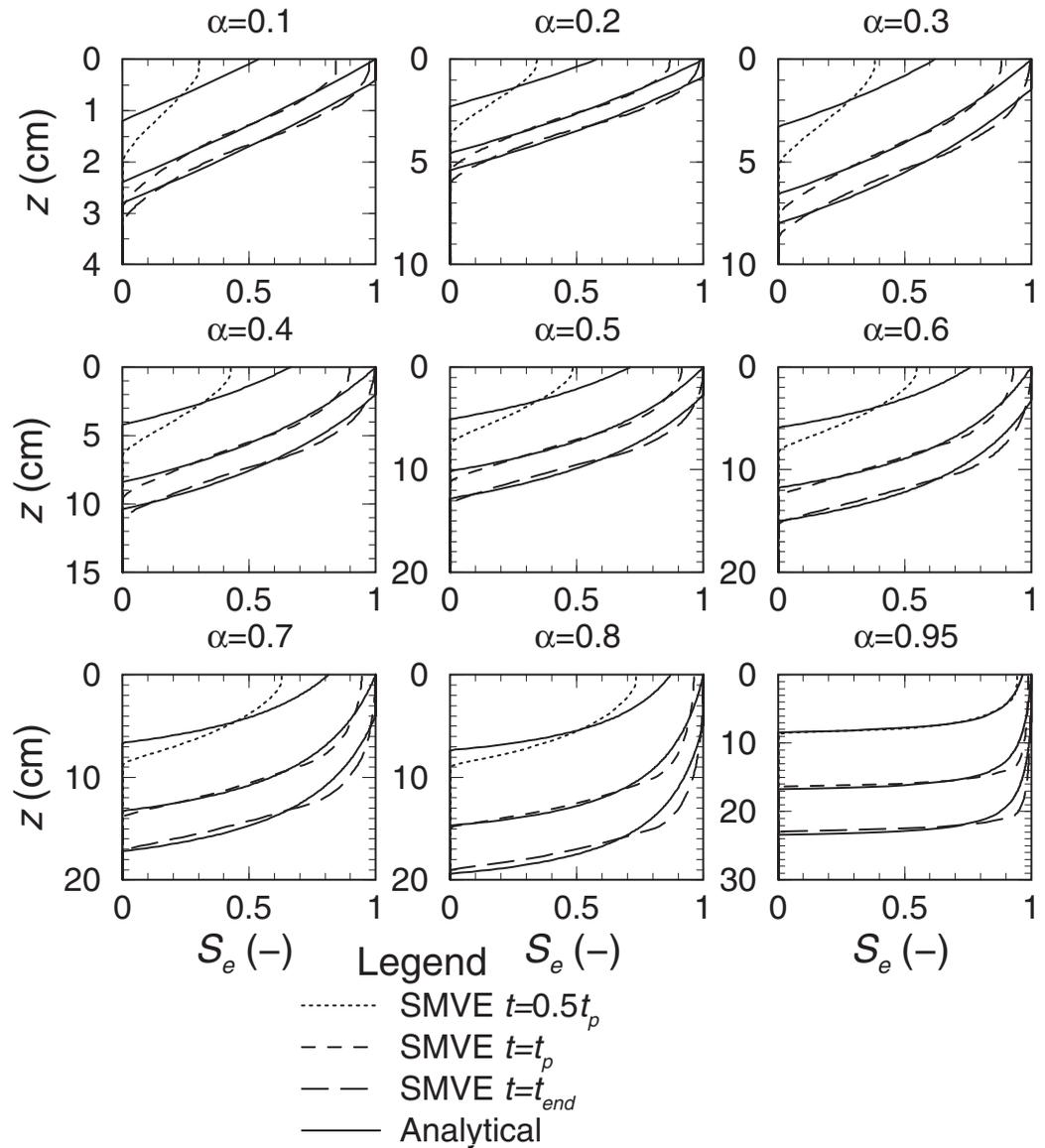


Figure 5. Results of tests of nonlinear water retention functions.

As before, the shape of the modeled wetting front profiles was evaluated using the NSE, PBIAS, and RMSE statistical measures. Those results are listed in Table 4.

Table 3. Differences in Cumulative Infiltration During Tests With Nonlinear Soil Water Retention Function

| α | $t = 0.5t_p$ | $t = t_p$ | $t = t_{end}$ |
|----------|--------------|-----------|---------------|
| 0.1 | -0.58% | -0.29% | -0.19% |
| 0.2 | -0.37% | -0.21% | -0.16% |
| 0.3 | -0.25% | -0.15% | -0.14% |
| 0.4 | -0.22% | -0.14% | -0.11% |
| 0.5 | -0.18% | -0.12% | -0.09% |
| 0.6 | -0.13% | -0.10% | -0.07% |
| 0.7 | -0.08% | -0.07% | -0.04% |
| 0.8 | -0.07% | -0.03% | -0.03% |
| 0.95 | -0.04% | 0.03% | 0.03% |

The ability of the SMVE advection-like term to predict wetting front shape compared to the case of the nonlinear law analytical solution is relatively poor for smaller values of parameter α at time $t = 0.5 t_p$, but quite good at later times. In the case of the largest parameter $\alpha = 0.95$, the SMVE profile starts out quite similar to the analytical solution, but diverges over time. Looking at the results in Figure 5, however, the SMVE wetting front profiles are not dissimilar from the analytical solution profiles. The PBIAS measures are all negative, indicating that the SMVE method on average under-

Table 4. Statistical Measures of Simulated Wetting Front Shape in Nonlinear Test, for Different Values of the Soil Water Constitutive Relation Parameter α

| α | NSE | | | PBIAS (%) | | | RMSE (cm) | | |
|----------|--------------|-----------|---------------|--------------|-----------|---------------|--------------|-----------|---------------|
| | $t = 0.5t_p$ | $t = t_p$ | $t = t_{end}$ | $t = 0.5t_p$ | $t = t_p$ | $t = t_{end}$ | $t = 0.5t_p$ | $t = t_p$ | $t = t_{end}$ |
| 0.1 | -2.03 | 0.97 | 0.98 | -22.37 | -2.44 | -0.28 | 0.30 | 0.10 | 0.09 |
| 0.2 | -1.83 | 0.96 | 0.98 | -21.38 | -1.42 | -0.66 | 0.58 | 0.21 | 0.17 |
| 0.3 | -1.36 | 0.98 | 0.97 | -16.91 | -1.44 | -0.48 | 0.80 | 0.24 | 0.30 |
| 0.4 | -0.95 | 0.98 | 0.97 | -13.10 | -1.38 | -1.15 | 0.93 | 0.31 | 0.40 |
| 0.5 | -0.64 | 0.98 | 0.95 | -10.91 | -1.29 | -0.46 | 1.03 | 0.33 | 0.70 |
| 0.6 | -0.25 | 0.98 | 0.93 | -7.67 | -1.66 | -1.57 | 1.03 | 0.41 | 0.90 |
| 0.7 | 0.11 | 0.96 | 0.91 | -3.56 | -2.56 | -3.06 | 1.00 | 0.58 | 1.19 |
| 0.8 | 0.44 | 0.93 | 0.87 | 2.65 | -4.78 | -5.12 | 0.93 | 0.89 | 1.62 |
| 0.95 | 0.99 | 0.72 | 0.67 | -0.30 | -13.74 | -7.58 | 0.18 | 1.89 | 2.91 |

estimates the depth to the wetting front. However, just like in the case of the power law test, the cumulative infiltration values listed in Table 3 indicate a maximum absolute error of less than 1%, with seven of the nine α values tested having less than 0.25% absolute cumulative infiltration error. For the smallest values of α tested, the RMSE decreased with increasing time. When $\alpha < 0.95$, the RMSE decreased as t increased to ponding time t_p then increased thereafter. The largest error in cumulative infiltration, 0.58% occurs when $\alpha = 0.1$, which represents a water retention function that is much too linear to represent a real soil. For $\alpha = 0.95$, the value that produces water retention functions that are the most similar to real soils, cumulative infiltration errors range from 0.03% to -0.04% .

6. Discussion

Maximum differences in cumulative infiltration in both tests ranged from -0.68 to 0.58% . This indicates that despite differences in the shapes of the wetting front profiles, the area behind the wetting front curves tended to be the very nearly same in both the analytical solution and the finite moisture-content solution of the SMVE advection-like term. The shape of the wetting fronts from the SMVE-FMC simulation were different compared to analytical solutions of both the power law and the nonlinear soil water constitutive relations. This difference was due to the fact that the SMVE-FMC solution neglects the diffusive flux due to the profile of the capillary head along the wetting front. However, neglecting the SMVE diffusion-like term in the case of the nonlinear constitutive relations resulted in errors in cumulative infiltration that were less than 0.05% in the case of $\alpha = 0.95$, which represents more realistic soil water retention characteristics. When α was small (0.1 and 0.2), the exact moisture content profiles are straight lines. In the power law case, wetting front profile shape agreement was better for larger values of n , and quite close for $n > 5$. In general, the SMVE solution is valid for any monotonic set of soil water constitutive relations, including those that represent subgrid variability in soil moisture [Qu *et al.*, 2015].

Comparison of numerical efficiency was not possible in this study because the analytical solution required no numerical solution. However, the SMVE advection-like term converted into an ODE and may be solved using a host of efficient ODE numerical solvers. Furthermore, solution is possible in a finite moisture-content discretization without actual $\Delta\theta$ bins by employing a vector solution that employs a finite Δz such as 1 cm. The vector stores only the number of bins that would contain water if there were actually bins in each Δz increment. This vector solution is 30 – 150 times faster than HYDRUS-1D depending on the degree of linearization applied in the HYDRUS-1D solution algorithm [Seo *et al.*, 2014].

Because we compared against analytical solutions in this study, we were unable to evaluate the ability of the advection-like term of the SMVE solved using the finite moisture-content method to simulate other vadose zone flows such as falling slugs or capillary groundwater dynamics. The ability of the solution to simulate falling slugs was demonstrated in Ogden *et al.* [2015a], while the response of the capillary groundwater to water table motion was demonstrated in numerical simulations compared to actual data from column tests by Ogden *et al.* [2015b].

There is nothing inherently mass conservative about equation (7) [Ogden *et al.*, 2015a]. Mass conservation is imposed on the simulation using a finite volume solution scheme that accurately detects collisions between

wetting fronts in bins. This solution accurately accounts for all water in the solution domain at all times during a simulation and guarantees conservation of mass, a major advantage that classical solutions of Richards' equation cannot claim.

The number of moisture-content bins required for optimal accuracy depends in part on soil texture [Talbot and Ogden, 2008, Table 3] but, more importantly, on the desired degree of resolution of the wetting front. Since one generally does not know the steepness of the wetting front before solving the model, accurate resolution in some problems may require adaptive refinement of the moisture-content grid, a possible subject for future improvements to the method. In the case of a near-surface groundwater table, most of the bins will be filled with water from the land-surface to the water table, and therefore require no computation of front displacements. In that case memory and computational requirements are both reduced, particularly for finer soil textures.

The first-principles derivation presented in Ogden *et al.* [2015a] was incomplete because of the properties of partial differential equations and appearance of another function in the enclosed derivation. The difference between the derivation by Ogden *et al.* [2015a] and the one presented herein is explained in the supporting information.

One limitation of the SMVE is that it is fundamentally a one-dimensional equation. Yu *et al.* [2012] proposed a higher-dimensional solution of the SMVE advection-like term, but work remains in that area. The second limitation arises because the method requires evaluation of no spatial derivatives, which is a good thing because the numerical evaluation of spatial derivatives with extremely nonlinear soil water retention functions is a major potential source of error in Richards' equation numerical solvers, but it requires that the soil properties be uniform in layers. There is no fundamental limit, however, on how thick or thin these layers may be, so continuously variable soil properties might be solvable using thin stacked SMVE solutions.

7. Conclusions

We have transformed the Richards [1931] equation into a new equation that contains separate advection-like and a diffusion-like flux terms. Because this equation predicts the velocity of discrete moisture contents, we call it the Soil Moisture Velocity Equation (SMVE). Neglecting the diffusion-like flux term, the SMVE advection-like flux term can be converted into an ordinary differential equation (ODE) using the method of lines and solved using a finite moisture-content (FMC) discretization [Talbot and Ogden, 2008; Ogden *et al.*, 2015a].

To determine the effect of neglecting the SMVE diffusion-like term, we compared the ODE solution of the SMVE advection-like term against two analytical solutions of the Richards [1931] equation developed by Ross and Parlange [1994]. Results showed that neglecting the diffusion-like term resulted in slightly different wetting front profile shapes, but that the cumulative infiltration values in each case tested differed from the exact solutions by less than 1%. This finding supports the notion that the SMVE advection-like flux term is sufficiently accurate as a replacement for the numerical solution of the one-dimensional Richards [1931] equation for calculating vertical fluxes of water in homogeneous soil layers. This finding also serves to verify that the omission of the diffusion-like flux term in the SMVE does not significantly affect the timing or amount of total infiltration flux because the mean of the diffusive flux term is very nearly zero for the cases tested, as demonstrated by the small differences in cumulative infiltration in the SMVE-FMC solution compared to the analytical solutions. Including the diffusion-like term would only be necessary if the objective was accurate simulation of wetting front profiles under all conditions.

The finite moisture-content solution of the SMVE advection-like term can replace the one-dimensional Richards [1931] equation in hyperresolution Earth system models and large-scale models of hydrology and land-atmosphere interaction. This solution allows accurate full two-way coupling of the groundwater through the vadose zone to the atmosphere using an efficient and reliable ODE solution methodology. The FMC solution is guaranteed to conserve mass and does not depend upon spatial discretization or linearization, something that up to now has eluded all who have tried to perform vadose zone simulations using numerical solutions of the one-dimensional Richards [1931] equation. Because the ODE solution of the advection-like term in the SMVE does not require calculation of spatial derivatives, it is not troubled by sharp wetting fronts or mathematical degeneracies associated with the numerical solution of Richards'

[1931] PDE, making it robust and reliable. Moreover, with computational efficiency and reliability, the ODE solution of the SMVE advection-like term is well suited for use in inverse problems such as when repeat remote sensing observations are used to infer soil hydraulic properties or soil moisture.

Acknowledgments

J.-Y. Parlange suggested the comparisons presented in this paper. This work was funded by NSF-EAR 1360384 and NSF-EPS 1135483, and the U.S. National Oceanic and Atmospheric Administration/National Weather Service/Office of Water Prediction, through UCAR subaward Z15-21991 to the first author. The data and source code for the model used in this paper are available at the following doi:10.15786/M22P4H.

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