Flow at Low Water Contents: A Simple Approach for Inverse Estimation of van Genuchten-Mualem Soil Hydraulic Parameters

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Abstract

The unsaturated soil hydraulic properties (the soil water characteristic and relative permeability curves) are key hydrodynamic parameters in the fields of soil science and civil engineering. Because of the strong dependency of these properties on water content, their determination is subject to considerable experimental and numerical problems. Difficulties increase when the soil approaches oven-dry conditions, a situation often encountered in arid and semi-arid areas. Moreover, computational costs of estimating the hydrodynamic properties can be relatively high also. After a short review of alternative modeling approaches for the hydraulic functions from saturation to oven-dryness, we present a theoretical-numerical approach, along with a relatively simple, robust and inexpensive experimental method for inverse determination of van Genuchten/Mualem soil hydraulic parameters. For gravimetric water contents greater than 0.04, numeral results agreed well with experimental data, while some discrepancies were observed at very low water contents.

1. Introduction

The process of water flow in soils has been the focus of intensive research in the fields of agronomy, hydrology and geomechanics. The amount and energy status of water in a soil can affect considerably the soil hydraulic properties. While knowledge of the two extreme states of water in a soil (saturated and very dry conditions) seems well advanced, the unsaturated state at medium to low water contents deserves further investigation. This condition is usually encountered in soil surface layers where strong interactions occur between soil and roots, microorganisms or building foundations. In arid and semi-arid zones, precise knowledge of physical flow processes at low water contents would allow development of more effective tools for water resources management.

The Richards equation is commonly used to describe water flow in the unsaturated zone of soils. Other formulations based on thermodynamics (Fremond and Nicolas, 1990) and/or the thermodynamics of irreversible processes (Bénet, 1981) lead to similar equations. Application of these equations in all cases requires initial and boundary conditions, as well as relationships between the gravimetric or volumetric water content (w in kg.kg^{-1}, and θ in m^3.m^{-3}, respectively) and the water flow rate. One can show that the suction or matric potential ψ (in Pa) and the matric head h (in m), both widely used in soil hydrology, are closely related to the chemical potential μ (J.kg^{-1}) (Bénet et al., 2012). The relationship between matric potential, chemical potential and matric head is given by $\mu=\psi/\rho_w=gh$, where ρ_w is the density of water, taken as 1000 kg.m^{-3}, and g the acceleration of gravity (m.s^{-2}). These relationships reflecting the soil hydraulic properties are conventionally expressed using two functions, namely the water retention function denoted by $w(\mu)$ and the hydraulic conductivity function $K(\mu)$ or $K(w)$. Additional processes may be included in the flow equation such as liquid-gas phase change (or evaporation), which is especially in arid regions.

All of the above functions and processes must be known from saturation to oven-dry conditions where measurements are especially challenging (Sakai et al., 2009). Physical and technical difficulties include possible cavitation of tensiometers (limiting their use up to about 80 J.kg^{-1}) and lack of continuity in the liquid phase of the soil when a saturated porous plate is used beyond 500 J.kg^{-1} (e.g., using the axis translation procedure as implemented by Baker and Frydman, 2009). In addition, acquisition of the data can be very time consuming and costly. For these reasons most studies are limited to situations between saturation and some intermediate state of soil water, corresponding to the range of operation of the most common experimental devices (Sakai et al., 2009; Fujimaki and Inoue, 2003; Fujimaki et al., 2004).

Inverse methods are now increasingly used to identify the hydraulic properties of unsaturated porous media. They offer a very flexible approach by allowing a range of numerical optimization algorithms (e.g., Levenberg-Marquart, conjugate gradient methods, genetic algorithms and neural network approaches). In soil hydrology, the approach generally used for inverse problems is solution of the Richards equation in conjunction with some infiltration/drainage or evaporation/condensation experiment (Durner et al., 1999; Fujimaki et al, 2004; Peters and Durner, 2008; Schindler et al., 2010; Sakai et al., 2009). A major difficulty of inverse problems is to find analytical or empirical models that accurately represent the hydraulic properties at very low water contents.

In this paper, we first review the problem of obtaining accurate descriptions of the soil hydraulic properties (the soil water characteristic and relative hydraulic conductivity curves) over the full range of water contents, but especially at relatively low water contents. The soil water characteristic curve is a representation of the relationship between soil water suction and water content. For suction ψ (Pa), we prefer to use the equivalent concept of water chemical potential μ (J.kg^{-1}), which provides a link between the physics of water in porous media and thermodynamically open systems. We next propose a theoretical-numerical model for isothermal water flow, which will be used in the inverse problem formulation. The selected state variables are the gravimetric water content, w, and the water vapor pressure, p_v. A simple, robust and very cheap experimental method for the inverse determination of the soil hydraulic properties is then presented. The soil hydraulic functions in this study are based on the van Genuchten model (1980) for the soil water characteristic and the van Genuchten (1980) - Mualem (1976) model for the unsaturated hydraulic conductivity. The ROSETTA code (Schaap et al., 2001) is further used to provide initial estimates of the model parameters. Various scenarios with regard to the residual water content, w_r, Mualem's tortuosity parameter, L, and the saturated hydraulic conductivity, K_{sat}, will be simulated and discussed.

2. Characterization of Soil Hydraulic Properties at Low Water Contents

2.1. The Soil Water Characteristic

Despite the relatively small amounts of water retained, accurate representation of soil water characteristic curves at the dry end is important for modeling biological processes including plant water uptake and microbial activity in arid environments (Tuller and Or, 2005). Accurate measurement over the full range of water contents is a delicate task. Most or all methods for measuring the water potential have limitations, especially at intermediate and very low values of the water content (its pendular and hygroscopic states). Very often the curve is completed by extrapolation, which can lead to instabilities in numerical codes (Lu et al, 2008). Experimental methods (infiltration and/or drainage, evaporation and condensation) associated with inverse problems also suffer from shortcomings, including in the instrumental devices, and are mostly robust only at the higher water contents (i.e., the funicular state) where the liquid phase is continuous. All this raises the question of the validity at low water contents of the matric head - water content relationship, h - θ, usually a key function to describe the physics of unsaturated flow. Indeed, this range of the water content comprises the pendular state where the liquid and vapor phases presumably are discontinuous, and the hygroscopic state where only the gas phase is continuous, while water is being strongly adsorbed onto the solid phase. This is why we prefer the use of the water chemical potential to describe the movement of water in all of its states. One of the fundamental properties of the chemical potential stipulates that at local thermodynamic equilibrium, the potential of a component present in two phases should be the same (Callen, 1985). Experimentally well-defined methods (e.g., Bénet et al., 2012) should apply to all important parts of the soil water characteristic curve, from saturation to oven dryness.

The models most commonly used in the literature to represent the soil water characteristic curve (Brooks and Corey, 1964; van Genuchten, 1980) often fail to reproduce experimental data at very low water contents (Sakai et al., 2009). Many researchers therefore developed new models or extended existing models to the full range of water contents. Campbell and Shiozawa (1992) used data at very high chemical potentials (in absolute value) to establish an equation reflecting the phenomenon of water adsorption on the surface of particles in the soil matrix. They modified the model of van Genuchten (1980) to improve the calibration of data at low water contents. The adsorption equation (Campbell and Shiozawa, 1992) was used later also by others (e.g., Fayer and Simmons, 1995; Khlosi et al., 2006) as an additional correction to the classical models at the low water contents. Fredlund and Xing (1994) opted for a different mathematical expression to better fit experimental data in this range. Junction models are now also available (e.g., Rossi and Nimmo, 1994; Webb, 2000; Zhang et al., 2011). Recent evaluations have highlighted the strengths and weaknesses of the various models. For example, Sillers and Fredlund (2001) noted that the Fayer and Simmons (1995) correction of van Genuchten's (1980) soil water characteristic model with m = 1.0 gave excellent results for about 200 soils from the USDA database over the entire range of moisture contents, while avoiding the controversial concept of residual water content. Using data from 137 soils of the UNSODA database, Khlosi et al. (2008) compared eight analytical models describing the complete soil water characteristic curve. They found that the model of Khlosi et al. (2006) with four fitting parameters was most consistent for soils covering a broad range of densities, organic matter contents and textures.

2.2. *The Unsaturated Hydraulic Conductivity*

Unlike the soil water characteristic curve, very few studies have been devoted to the hydraulic conductivity over the full range of water contents (Zhang, 2011). One problem involves the physical processes that govern the flow of water at low water contents. While capillary models based on theories by Purcell (1949), Childs and Collis (1950), Burdine (1953), Kunze (1968) and Mualem (1976) for estimating the unsaturated hydraulic conductivity are generally fairly accurate at high water contents, they often underestimate the permeability at low water contents (Sakai et al. 2009). Hydraulic conductivity expressions that have been validated over the full range of water contents often are relatively complex and sometimes difficult to use within an inverse optimization program. As for the physical flow phenomena at low water contents, Tuller and Or (2001), Peters and Durner (2008) and Zhang (2011) use the concepts of film flow at low water contents to establish hydraulic conductivity models over the full range of water contents. The model of Tuller and Or (2001) is mathematically very complex and not easily associated with one of the classical models for the soil-water characteristic curve. Those of Peters and Durner (2008) and Zhang (2011) add an extra term accounting for capillary flow according to the theories of Mualem (1976) and Burdine (1953), and another term describing film flow around solid particles in the soil matrix. However, some of these models remain very complex, especially when used in an inverse procedure.

3. Theoretical-Numerical Model for Water Flow in Arid Soils

A natural soil can be idealized as a triphasic porous medium by considering a solid, a liquid and a gaseous phase, with the gaseous phase consisting of two components: dry air and water vapor. From an experimental point of view, appropriate state variables for water flow modeling are the gravimetric water content, w, defined as the ratio between the apparent mass densities of liquid, ρ_l, and solid ρ_s (i.e., $w=\rho_l/\rho_s$), and the vapor partial pressure of the gas phase, p_v (Pa) linked to the apparent density of vapor, ρ_v, through the ideal gas law:

$$p_v = \frac{\rho_v}{\phi_g}\frac{RT}{M_w} \tag{1}$$

where R (J.kg^{-1}) is the ideal gas constant and M_w (kg.mol^{-1}) the molar mass of water. The volume fraction of the gas phase ϕ_g is related to the water content w by:

$$\phi_g = \frac{V_g}{V} = 1 - \frac{\rho_s}{\rho_s^*} - w\frac{\rho_s}{\rho_l^*} \tag{2}$$

Three elementary processes are considered: liquid flow governed by capillary and gravity effects, vapor diffusion in the gas phase, and liquid-gas phase changes of water. The main assumptions are that the temperature is uniform and constant, the solid skeleton is rigid, the total gas pressure is constant and uniform, and hence also that convective flow in the gas phase is negligible.

Fundamental mass balance equations for water in liquid and gas phases are then written as:

$$\rho_s \frac{\partial w}{\partial t} + \nabla.(\rho_l \mathbf{v}_l) = -\hat{\rho} \tag{3}$$

$$\frac{M_w}{RT}\frac{\partial}{\partial t}(\phi_g p_v) + \nabla.\mathbf{J}_v = +\hat{\rho} \tag{4}$$

The liquid filtration flux, denoted by $\rho_l \mathbf{v}_l$ in Equation (3) is described with Darcy's law extended to unsaturated conditions. Extension of the above description to very low water contents is questionable since the concept of liquid pressure is meaningless (Nitao and Bear, 1996). An alternative proposed by Bénet et al. (2012) is to rely on the chemical potential, which is defined over the full range of water contents. This thermodynamic potential is a function of the water content described by the soil-water retention curve obtained by merging measurements using classical tensiometry and sorption isotherms. Therefore, water flow can be governed by the equation:

$$\rho_l \mathbf{v}_l = -K_{sat} k_r \frac{\rho_l^*}{g}(\nabla \mu_l - \mathbf{g}) \tag{5}$$

where μ_l (J.kg^{-1}) is the mass chemical potential of liquid water, $\mathbf{g}$ (m.s^{-2}) is the gravity acceleration vector, k_r is the relative permeability function and K_{sat} (m.s^{-1}) the hydraulic conductivity at saturation. The mass density of water ρ_l^* is taken to be 1000 kg.m^{-1}.

The vapor diffusion flux, denote by $\mathbf{J}_v$ in Equation (4), is classically described using a first-order Fick's law of the form:

$$\mathbf{J}_v = D_{vs} \nabla \rho_v^* \tag{6}$$

in which D_{vs} is the effective vapor diffusion coefficient in the soil:

$$D_{vs} = \tau \phi_g D_{va} \tag{7}$$

where τ is the tortuosity, which can be described using functions given by Penman (1940), Millington and Quirck (1961) or Moldrup et al. (1997), and D_{va} the free diffusion coefficient of vapor in air. Standard correlations give a value of 26.1×10^{-6} m.s^{-2} for D_{va} at 30°C.

From thermodynamic considerations of liquid-gas phase changes, it can be shown that the volumetric rate of phase change is proportional to the chemical potential difference of water between the liquid and vapor states. A detailed theoretical development of this phase change has been given by Bénet et al., (2009).

The nonlinear equations (3) and (4) are strongly coupled through the phase change term $\hat{\rho}$, as well as through the soil physical characteristics that depend on the water content: $\phi_g(w)$, $D_{vs}(w)$, and $k_r(w)$. The governing equations were discretized using a finite-volume formulation on a one-dimensional regular mesh, with the unknowns w and p_v located at the center of grid blocks. A first-order upstream scheme was used to describe the convective term appearing in liquid mass balance Equation (3). Temporal integration was performed based on a fully implicit scheme to ensure numerical stability. Nonlinearities were dealt with by using a Newton-Raphson method which produced accurate convergence with relatively moderate time steps.

4. Materials and Methods

4.1. Morphological Characteristics and Soil Moisture

The material under investigation is a natural soil from Nasso, Burkina-Faso. The soil sample was taken from the top layer of soil (0-30 cm depth). The analysis by dry sieving after washing (standard NF P94-056) for particles having diameters greater than 80 µm and a sedimentation analysis (standard NF P94-057) for smaller particles, indicated that the soil contained 95% sand, 2% silt and 3% clay (USDA classification). Soil texture is hence sand. The dry soil density measured at the site gave an average value of 1688 $kg.m^{-3}$. Points of the soil water characteristic (desorption data) were obtained by combining two methods: using a pressure plate apparatus at constant temperature (30°C) for water in the funicular state (saturations up to μ = -500 $J.kg^{-1}$) and a desorption device (using saturated solutions at equilibrium) to complete the curve in the hygroscopic state (from -5000 to -3×10^5 $J.kg^{-1}$). Figure 1 shows the measured data as well as the relationship between the chemical potential and the water content based on the model of van Genuchten (1980) as identified using the RETC code of van Genuchten et al. (1991).

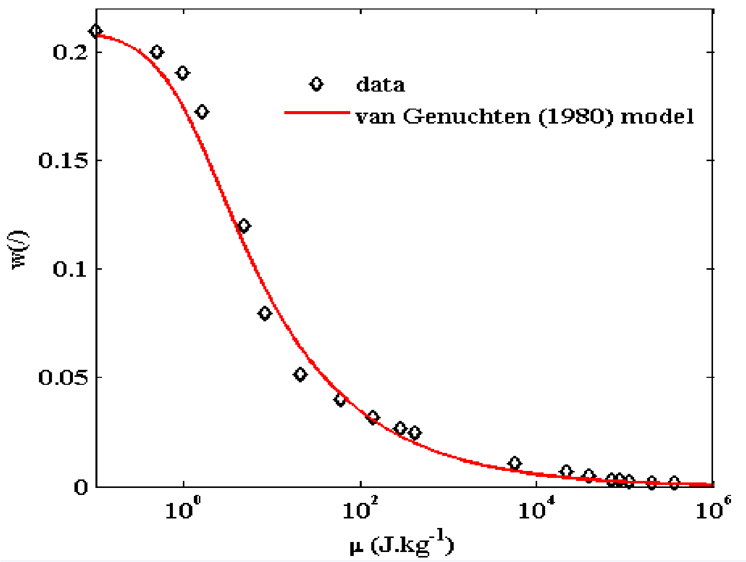

Figure 1. Measured and fitted soil water characteristic curves (gravimetric water content, w, as a function of the chemical potential, μ).

4.2. Measured Water Content Profiles

The objective of the experimental study was to establish profiles of water content in a homogeneous soil column. The upper half of the PVC column used for this purpose (20 cm high and 7.5 cm inner diameter) was packed with soil having a desired initial gravimetric water content of 0.06, and the lower half with soil having a gravimetric water content of 0.02. Both parts of the column were compacted to the field-measured dry density. The sealing ends of the columns were coated with a thick plastic film. Crafted columns were stored in a thermo-regulated chamber. Evaporative phenomena were negligible. The mass of the column was assumed to be constant. The experiment consisted in a redistribution of water on both sides of the interface due to the gradient of the moisture content (or chemical potential). A destructive method was used for measurement of gravimetric water contents by weighting after oven-drying at 105°C for 48 hours. The soil columns for this purpose were sliced using a mechanical device to determine the distributions of the water content along the column at given time intervals. The mechanical device permitted slices of soil of only 5 mm thick. Ideal conditions of the experiment were such that only the physical phenomenon of water flow in the column occurred (e.g., flow of water in the liquid phase from the top part). Phase changes could be neglected since air within the column was presumably saturated.

4.3. Inverse Analysis

The inverse analysis was based on solutions of the theoretical model given by Equations (3) and (4) using a nonlinear Newton-Raphson method. The chemical potential as a function of the water content was described using the model van Genuchten (1980) and the relative permeability function using the van Genuchten (1980) - Mualem (1976) equation as follows:

$$S_e = \frac{w(\mu) - w_r}{w_{sat} - w_r} = \left[1 + \left(|\alpha\mu|\right)^n\right]^{-m} \quad (8)$$

$$k_r(S_e) = S_e^L \left[1 - \left(1 - S_e^{1/m}\right)^m\right]^2 \quad (9)$$

where w_r and w_{sat} are the residual and saturated gravimetric water contents, respectively, α (> 0 in kg.J^{-1}), n (> 1) and L are fitting parameters, m=1-1/n as suggested by van Genuchten and Nielsen (1985), and S_e is effective saturation. In this study we selected the above original van Genuchten equations rather than the complicated modified expressions advocated by Schaap and van Genuchten (2006).

Two minimization programs were used next in the inverse analysis to find optimal hydraulic parameter values based on obtaining the minimum average squared difference between measured and calculated values: one based on the Levenberg-Marquardt (1963) algorithm, and another one using the Nelder-Mead Downhill Simplex method (Nelder and Mead, 1965). All optimizations produced a value of zero for the residual water content (w_r = 0), while the saturated water contents w_{sat} was fixed at 0.208 kg.kg^{-1} as estimated from the measured porosity of the soil. Since laboratory saturated permeability tests (rigid-wall or flexible-wall permeameters) often show considerable errors (e.g., Chapuis, 2012) with predicted values sometime deviating considerably from measured values due to macroporosity or other effects (Schaap and Leij, 2000; Schaap and van Genuchten, 2006), we decided to keep K_{sat} as a free (adjustable) parameter in the inverse analysis.

Table 1. Assumed optimization scenarios and imposed parameter constraints

Scenario	Free parameters	Fixed parameters	Lower bond	Upper bound
S1	K_{sat} (m.s^{-1})	$w_r = 0$, α, n, $m = 1\text{-}1/n$, $L = 0.5$	10^{-10}	10^{-3}
S2	n, m, K_{sat} (m.s^{-1})	$w_r = 0$, α, $L = 0.5$	n>1, m>0	n<10, m<1
S3	K_{sat} (m.s^{-1})	$w_r = 0$, α, n, $m = 1\text{-}1/n$, $L = -6.5$	10^{-10}	10^{-3}
ROS	α, n, K_{sat} (m.s^{-1})	$w_r = 0$, $L = 0.5$	-//-	-//-

Several optimization scenarios were considered as summarized in Table 1. Scenario S1 corresponds to an optimization of the saturated permeability (K_{sat}) with the model parameters $w(\mu)$ deduced from the fitted soil water characteristic curve in Figure 1. Scenario S2 considered both m and K_{sat}, to be the optimization parameters. The parameter m in Equation (9) is in that case independent of n in Equation 8. In a third scenario, S3, following the work of Schaap and Leij (2000), Peters et al. (2011), Peters and Durner (2008) and Zhang (2011), we fixed L at a negative value (-6.5) and focused on the optimization of K_{sat}. The other parameters kept the values associated with Figure 1. In a fourth scenario, denoted ROS, we optimized all parameters of Equations 8 and 9. The initial values were estimated from textural properties and the density using the ROSETTA code (Schaap and al., 2001). Parameter constraints were further introduced to ensure realistic physical descriptions of the hydraulic functions. Inspired by the work of van Genuchten and Nielsen (1985); Ippisch et al. (2006) and Peters et al. (2011), we used the following constraints: $1<n<10$, $0<m<1$, and $0<\alpha<15$. Following Schaap and Leij (2000) and Schaap and van Genuchten (2006), we further imposed the constraint $10^{-10}<K_{sat}<10^{-3}$ on the saturated hydraulic conductivity of our sandy soil.

5. Results and Discussion

Table 2 summarizes the estimated values for optimization scenarios (S1, S2, S3, ROS), including values of the Root Mean Square Error (RMSE). Figures 2 and 3 show the experimental and simulated profiles according to the scenarios presented in Table 1. Figure 2 is for scenario S1, while Figure 3 shows results for all scenarios at different times (1, 3, 5 and 13 days).

Table 2: Optimized values of van Genuchten/Mualem model parameters.

Scenario	α	n	m	K_{sat}	RMSE
	kg.J^{-1}	-	-	m.s^{-1}	
S1	0.9527	1.3922	1- 1/n	$3.6946.10^{-5}$	0.002652
S2	0.9527	1.3922	0.6288	$2.3698.10^{-7}$	0.002068
S3	0.9527	1.3922	1- 1/n	10^{-10} +	0.006482
ROS	13.1034	1.0 *	1- 1/n	$4.3277.10^{-5}$	0.002286

+ minimum limit imposed

* minimum limit imposed, $n_{opt} = 0.86735$

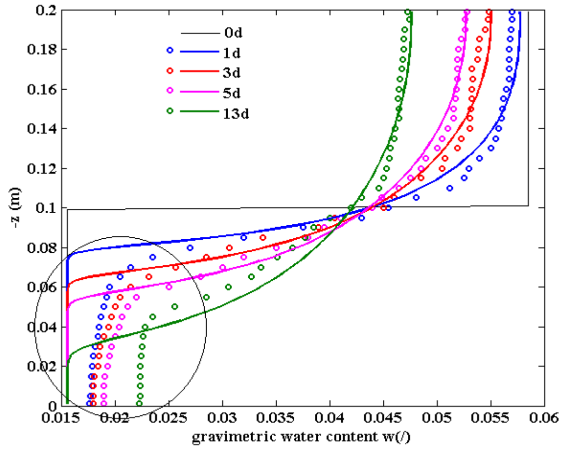

Figure 2. Experimental and simulated water content profiles for scenario S1.

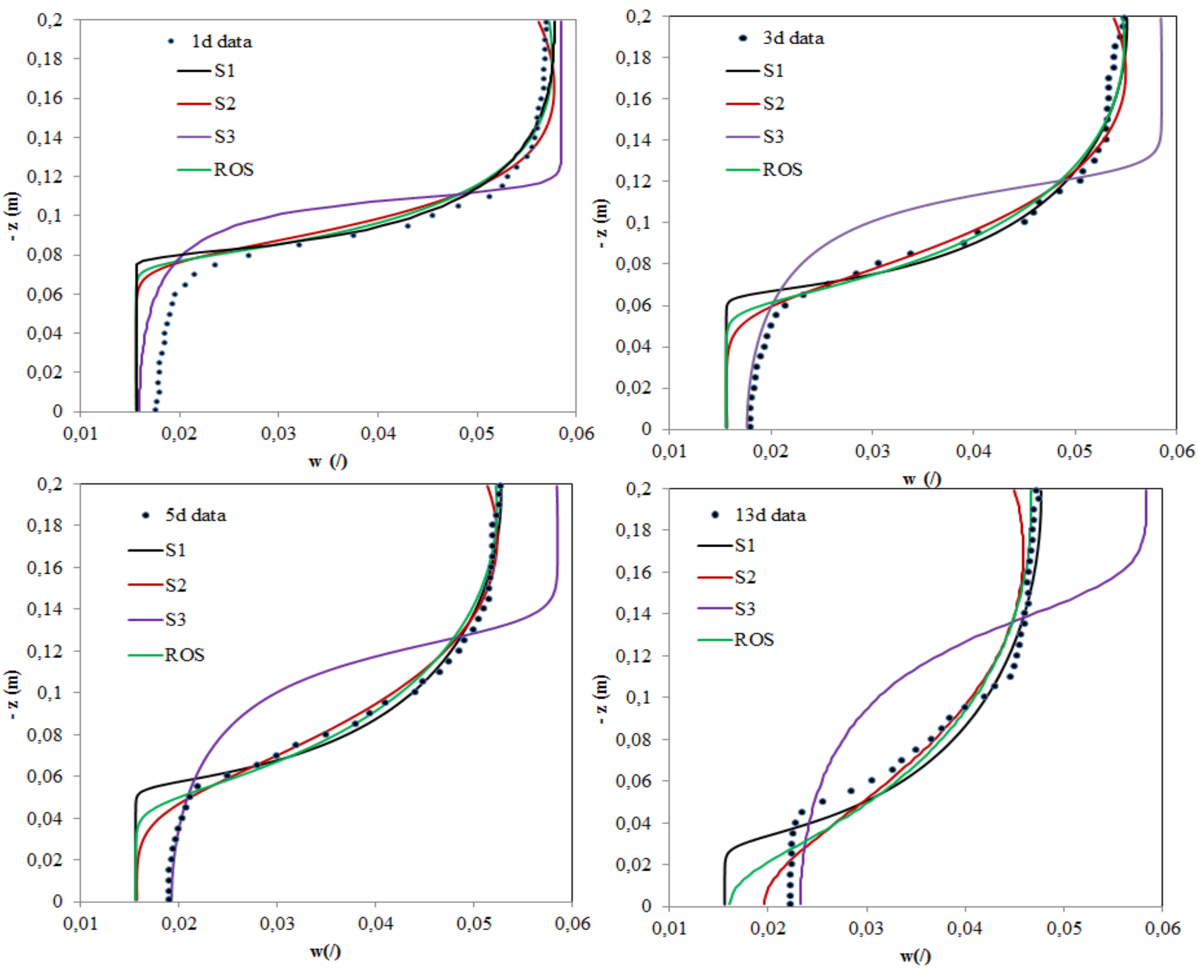

Figure 3. Experimental and simulated water content profiles for optimization scenarios S1, S2, S3, and ROS at different times (1, 3, 5 and 13 days).

The results presented in Table 2 and Figures 2 and 3 show that the inverse analysis in conjunction with the assumed numerical model (section 3) leads to a good match with the experimental data. The inverse procedure based on the Levenberg Marquart method was found to be quite robust by producing unique solutions. The computational time depended on the number of parameters to be optimized and the invoked initial values. The Nelder-Mead method (1985), on the other hand, was found to be very time-consuming.

Except for case S3, all scenarios using the van Genuchten model for $w(\mu)$ and the van Genuchten-Mualem model for the unsaturated hydraulic conductivity accurately described the flow of water at relatively high water contents. Below 0.03, however, significant discrepancies are apparent in Figure 2. When the parameter n of Equation 8 was optimized along with m (kept independent of n) and K_{sat} (i.e., scenario S2), the inverse analysis gave the best results in terms of yielding the lowest value of RMSE. However, the optimized value for K_{sat} (2.3698×10^{-7} ms^{-1}) was very small compared to typical values for a sandy soil, as can be observed in the work of Schaap and Leij (2000). Taking into account the textural properties of the soil, optimizing all parameters (α, n, m = 1-1/n, K_{sat}) and using initial estimates provided by ROSETTA (Schaap et al., 2001) produced excellent results (RMSE = 0.002286). This case may well prove the most promising for characterizing the hydraulic properties of unsaturated soils. The cost of the method is very small considering the simplicity of the experimental method, including the use of initial estimates as predicted with ROSETTA from soil texture.

Optimizing K_{sat} according to scenario S3 produced the lowest value of the saturated hydraulic conductivity ($K_{sat} = 10^{-10}$ ms^{-1}), while only a fair match was obtained at the lower water contents. This case also failed to reproduce the observed gradients in the moisture profile in the centre of the column at intermediate water contents.

6. Conclusion

Determining the unsaturated soil hydraulic properties at very low water contents is still a major challenge. Existing numerical and experimental methods have many limitations in the very dry range. The theoretical model we proposed in this paper is based on the chemical potential, which provides a fundamental thermodynamic link between the physics of water flow in porous media and the thermodynamics of open systems. A numerical inverse procedure was developed to identify the parameters associated with the models of van Genuchten (1980) for the soil-water characteristic curve and the van Genuchten (1980) - Mualem (1976) formulation for the unsaturated hydraulic conductivity. Experimental water content profiles were obtained using a very simple experimental setup. The optimized parameters remained within their physical limits, in agreement with literature values. They closely described the results as shown by relatively small RMSE values. However, discrepancies were still observed at very low water contents. An alternative is to rely on the general model of van Genuchten and Nielsen (1985) with independent m and n values, which gives more flexibility to match the experimental results in the low water content range.

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