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Improving prediction of hydraulic conductivity by constraining capillary bundle models to a maximum pore size

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ABSTRACT

The prediction of unsaturated hydraulic conductivity from the soil water retention curve by pore-bundle models is a cost-effective and widely applied technique. One problem for conductivity predictions from retention functions with continuous derivatives, i.e. continuous water capacity functions, is that the hydraulic conductivity curve exhibits a sharp drop close to water saturation if the pore-size distribution is wide. So far this artifact has been ignored or removed by introducing an explicit air-entry value into the capillary saturation function. However, this correction leads to a retention function which is not continuously differentiable. We present a new parameterization of the hydraulic properties which uses the original saturation function (e.g. of van Genuchten) and introduces a maximum pore radius only in the pore-bundle model. In contrast to models using an explicit air entry, the resulting conductivity function is smooth and increases monotonically close to saturation. The model concept can easily be applied to any combination of retention curve and pore-bundle model. We derive closed-form expressions for the unimodal and multimodal van Genuchten–Mualem models and apply the model concept to curve fitting and inverse modeling of a transient outflow experiment. Since the new model retains the smoothness and continuous differentiability of the retention model and eliminates the sharp drop in conductivity close to saturation, the resulting hydraulic functions are physically more reasonable and ideal for numerical simulations with the Richards equation or multiphase flow models.

1. Introduction

Modeling water fluxes in soils with the Richards equation requires accurate estimates of the soil hydraulic properties. In contrast to the water retention curve (WRC), which can be well determined in the laboratory by different methods [10], the determination of the hydraulic conductivity curve (HCC) is time-consuming and costly. For this reason, the prediction of hydraulic conductivity from the WRC by capillary bundle models is attractive and applied widely although the underlying theory and assumptions are not necessarily valid for all soils [15]. Apart from a correct theory to derive the HCC from the WRC, an accurate prediction of the HCC requires a mathematical description of the WRC. The choice of a model for the WRC can exert a strong influence on the predicted HCC and this influence is most pronounced close to water saturation, where the HCC is very sensitive to small changes in water retention [8,30]. If a smooth S-shaped function like the one proposed by van Genuchten [29] is used to parameterize the WRC of a fine-textured soil or a soil with a wide pore-size distribution, the HCC may exhibit an abrupt drop close to saturation. This drop (i) leads to a strong underprediction of hydraulic conductivity close to saturation if the prediction of the HCC is based on the measured saturated hydraulic conductivity [32] and (ii) negatively affects the performance of numerical solvers, i.e. their stability and accuracy at the transition between saturated and unsaturated conditions [18,32]. This issue has been approached before by (i) shifting the entire pore-size distribution by an air-entry value [19], (ii) truncating the pore-size distribution [20] or (iii) introducing an explicit air-entry pressure into the van Genuchten model [18, 31,32]. The third approach is the most widely applied because it allows a closed-form equation for the HCC in the case of the van Genuchten–Mualem model. It effectively eliminates the drop in the HCC near saturation and the related adverse effects on the behavior of numerical solvers of the Richards equation [18,32]. Although it has been argued that the introduction of an air-entry value reflects the fact that a maximum pore-size exists in any soil [18], other authors point out that limitations in measurement abilities impede the accurate determination of this entry-pressure. In most studies, the model selected to parameterize the WRC extrapolates the soil water content which is measured at a suction exceeding the air-entry suction toward water

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saturation [30]. Furthermore, a smooth transition zone in the vicinity of the air-entry pressure is often observed for field-measured WRC [30]. The main disadvantage of the introduction of an explicit air-entry value into the retention model is, however, that the resulting WRC is no longer continuously differentiable, i.e. the soil water capacity function becomes discontinuous, which poses a challenge to numerical solvers of the Richards equation. This argument holds as well for other models of the WRC with an explicit-air-entry pressure, e.g. the model of Brooks and Corey [3], and was one of the reasons for seeking alternative smooth formulations for the WRC (e.g. [4]).

In the following, we suggest an alternative technique to solve the problem of a marked drop in the HCC close to saturation for wide pore-size distributions. In a nutshell we propose to not alter the WRC and thus to retain its smoothness and continuous differentiability, but to restrict the pore-size within the pore-bundle model for HCC prediction to a maximum value [7]. The model concept is illustrated for the capillary-bundle model of Mualem [21] applied to the unimodal and multimodal WRC of van Genuchten [8,29]. We derive closed-form expressions for the proposed modification and illustrate the practical use of the new model by (i) fitting a WRC to measured point data and comparing the prediction of the HCC with independent measurements, and (ii) inverse modeling of a multistep outflow experiment using numerical solutions of the Richards equation.

2. Theory

2.1. Review of current approaches

2.1.1. Capillary bundle models and the van Genuchten–Mualem model

In general, capillary bundle models can be written as [14]

$$K(S) = K_s S^{\tau} \left[\frac{\int_0^S h^{-u} ds}{\int_0^1 h^{-u} ds} \right]^v = K_s S^{\tau} \left[\frac{F(S)}{F(1)} \right]^v \quad (1)$$

where $K(S)$ [L/T] is the soil hydraulic conductivity as function of the effective saturation S [–], h [L] denotes the suction or absolute value of the pressure head, u, v, and τ are dimensionless parameters, and $F(S)$ is the closed-form or numerical solution of the integral. The values of the parameters u and v vary among different capillary-bundle models from the literature. For instance, $u = 2$ and $v = 1$ for Burdine's model [5] and $u = 1$ and $v = 2$ for Mualem's model [21] to which we will restrict the presentation in this article for the sake of brevity. The parameter τ is an empirical parameter accounting for the tortuosity and connectivity of the pore space which is commonly set to a value of 0.5 following Mualem [21]. Physically feasible values for different parameterizations of the WRC and Mualem's capillary bundle model were derived by [24,26].

One of the most popular choices for the parameterization of the saturation function is the van Genuchten equation [29]:

$$S(h) = [1 + (\alpha h)^n]^{-m} \quad (2)$$

where α [L^{-1}], n [–] and m [–] are shape parameters. The volumetric soil water content is calculated from Eq. (2) by the relation

$$\theta(h) = (\theta_s - \theta_r)S(h) + \theta_r \quad (3)$$

where θ_s [–] and θ_r [–] are the saturated and residual water contents, respectively. In most applications, the parameter m is computed from parameter n by the equation

$$m = 1 - \frac{1}{n} \quad (4)$$

because this reduces the number of parameters and ensures an analytical closed-form expression for $K(S)$ if Mualem's model is applied [29]. If Eqs. (2) and (4) are used in Eq. (1) in the case of $u = 1$ and $v = 2$, the closed-form expression $F(S)$ becomes:

$$F(S) = \int_0^S \frac{1}{h} ds = \alpha[1 - (1 - S^{1/m})^m] \quad (5)$$

and the equation to predict $K(S)$ becomes [29]:

$$K(S) = K_s S^{\tau}[1 - (1 - S^{1/m})^m]^2 \quad (6)$$

Eqs. (2)–(4) and (6) are jointly referred to as the van Genuchten–Mualem model (VGM). A well-known problem of Eq. (6) is that it predicts a relatively sharp drop in $K(S)$ close to saturation if the parameter n, which quantifies the width of the pore-size distribution, becomes smaller than 2. The mathematical reason for this is that

$$\lim_{h\to 0}\left(\frac{1}{h}\frac{dS}{dh}\right) = \lim_{h\to 0}\left(\frac{d^2S}{dh^2}\right) \quad (7)$$

is zero for $n > 2$, is finite for $n = 2$, and goes to infinity if $n < 2$ [18]. Unfortunately, many fine-textured soils exhibit n values smaller than 2 [23]. For example, from the 12 textural soil classes reported by [6] only sand and loamy sand have a value of n greater than 2. The physical reason for the misbehavior of Mualem's model for $n < 2$ is that the pore-size distribution inherent to the WRC predicts the occurrence of a small fraction of pores with radii r [L] much larger than a size representative for or even possible in real soils. Since capillary bundle models use Poiseuille's law for the calculation of $K(S)$, which states that $K \sim r^2$, the predicted occurrence of even an arbitrarily small fraction of water occupied by such large pores causes a severe drop in hydraulic conductivity close to saturation. This drop in $K(S)$ is unphysical and must be corrected.

2.1.2. Introduction of an explicit air entry value

To prevent the sharp conductivity drop at saturation, it has been proposed to introduce an explicit air-entry suction to the saturation function $S(h)$ [32]. This suction can be related to a maximum pore radius by the Young-Laplace equation. As shown by Ippisch et al. [18], the van Genuchten saturation function is then modified to:

$$S(h) = \begin{Bmatrix} \frac{1}{S_a}\left[1 + (\alpha h)^n\right]^{-m} & \text{if} \quad h > h_a \\ 1 & \text{if} \quad h \le h_a \end{Bmatrix} \quad (8)$$

where h_a [L] is the air-entry suction of the soil, and $S_a = S(h_a)$ [–]. By using Eq. (8) in Mualem's model one obtains the closed-form expression for the HCC [18]:

$$K(S) = \begin{Bmatrix} K_s S^{\tau}\left[\frac{1 - (1 - (S S_a)^{1/m})^m}{1 - \left(1 - S_a^{1/m}\right)^m}\right]^2 & \text{if} \quad h > h_a \\ K_s & \text{if} \quad h \le h_a \end{Bmatrix} \quad (9)$$

We will refer to the model given by Eqs. (3), (4), (8), and (9) as VGM-AE (AE for air-entry) in the remainder of this article. Note that this model was derived by Vogel et al. [32] but with slightly different terminology and that Ippisch et al. [18] have reformulated it in a more elegant way, which makes it easier to apply the concept to arbitrary saturation functions $S(h)$. Vogel et al. [32] have suggested to always use model Eqs. (8) and (9) if $n < 1.3$ and to choose h_a from the interval 1–4 cm to ensure that the overall impact on the WRC is insignificant while the drop in hydraulic conductivity near saturation is eliminated. The numerical advantages of the VGM-AE have been demonstrated for various infiltration conditions [32]. Ippisch et al. [18] have applied the model for inverse simulations of multistep outflow experiments and assessed its influence on parameter estimation.

In many practical situations, parameterizing the WRC with models assuming a unimodal pore-size distribution is problematic because it cannot provide an accurate description of experimental data. For this reason and because this model will be used in the application section, we additionally discuss the case of multimodal approaches