Comment on “A Modular Framework for Modeling Unsaturated Soil Hydraulic Properties Over the Full Moisture Range” by Weber et al.

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Abstract Weber et al. (2019) (W19 in the following) present a modular framework for parametrizing soil hydraulic properties. The W19 model framework is almost identical to the model system developed jointly by Peters (2013), Iden and Durner (2014), and Peters (2014), to which we will refer as PDI (“Peters-Durner-Iden”) model in the following. The primary goal of this comment is to uncover some inconsistencies of the W19 formulation. In the following, we (i) comment on the statement made by W19 regarding the number of parameters in the original PDI formulation, (ii) critically analyze the use of their function to parameterize the water retention curve (WRC), and (iii) show that, in contrast to the statement in W19, using their formulation of non-capillary hydraulic conductivity leads to systematic deviations from the physically based film-conductivity model developed by Tokunaga (2009).

1. Introduction

Weber et al. (2019) (W19 in the following) present a modular framework for parametrizing soil hydraulic properties. The W19 model framework is almost identical to the model system developed jointly by Peters (2013), Iden and Durner (2014), and Peters (2014), to which we will refer as PDI (“Peters-Durner-Iden”) model in the following. This is documented by the fact that the PDI model system is repeated in Equations 1–3 and 8–11 in W19. We note that there are many approaches to account for capillary and noncapillary storage and flow in soil hydraulic properties (e.g., Tuller and Or (2001), Lebeau and Konrad (2010), or Zhang (2011), however the model system presented in W19 resembles the PDI system, namely the linear superposition of a capillary and a noncapillary component of water retention function (Equations 1 and 2 in W19), the scaling approach for the capillary component (Equations 3 in W19), the linear superposition of a capillary, a noncapillary and an isothermal component of the hydraulic conductivity function (Equations 8 and 9 in W19) and the resulting mathematical formulation of the capillary bundle models (Equation 11 in W19, the limits of integration are wrong in Equations 10 and 11 in W19, though). Peters (2013) and Iden and Durner (2014) already compared the performance of two capillary saturation functions in the PDI, namely those of van Genuchten (1980) and Kosugi (1996). Peters (2014) derived closed-form equations for the soil hydraulic conductivity function for these cases and the bimodal retention curve of Durner (1994). Weber et al. (2017) used uni-, bi-, and tri-modal van Genuchten functions within the PDI to parametrize hydraulic properties of peat. More variants, including those saturation functions which require a numerical solution for the capillary conductivity function, can be found in Peters and Durner (2015). Any capillary and noncapillary saturation function as well as capillary and noncapillary conductivity function can be combined within this scheme, and isothermal vapor flow can easily be included in the conductivity function.

To our understanding, the novel part of W19 is the introduction of an alternative formulation for the noncapillary saturation function $S_{nc}$ ( ), whereas all other model equations and the model framework itself is already contained in the PDI model scheme. We acknowledge that the results of W19 confirm those of previous studies in which extended models of the hydraulic properties improved the description of experimental data over a wide range of suction (Lebeau & Konrad, 2010; Peters, 2013; Zhang, 2011, to only name a few).

The objective of this comment is not to compare the original PDI formulation with the version of W19 in terms of their ability to describe measured data. Neither do we aim to provide a full theoretical analysis of
the physics of noncapillary flow in porous media and their possible representation in hydraulic properties. Both the original PDI and the W19 version, are intended to be simple formulations to effectively describe the relevant storage and flow mechanisms. Neither PDI nor W19 do account for more complete theories like that of Tuller and Or (2001). The primary goal of this comment is to uncover some inconsistencies of the W19 formulation. In the following, we (i) comment on the statement made by W19 regarding the number of parameters in the original PDI formulation for \( S_{nc} \), (ii) critically analyze the use of their function \( S_{nc} \) to parameterize the water retention curve (WRC), and (iii) show that, in contrast to the statement in W19, using their formulation of \( S_{nc} \) for parametrizing noncapillary hydraulic conductivity leads to systematic deviations from the physically based film-conductivity model developed by Tokunaga (2009). Throughout this comment, we denote the absolute value of matric head, the suction or tension, by \( h \) (L), express it in cm, and denote its common logarithm as \( x = \log_{10}(h) \), which is equal to the pF introduced by Schofield (1935).

### 1.1. Number of Adjustable Parameters

W19 claim that in contrast to the PDI function for \( S_{nc} \), their model does not require an extra parameter and explicitly mention the parameter \( h_a \) (L) used in the PDI model in this context. While we acknowledge that this parameter is not necessary in the W19 model, we emphasize that Peters (2013) discussed different approaches to set (not to estimate) \( h_a \) on the basis of the parameters of the capillary saturation function. For the saturation functions of van Genuchten (1980) and Kosugi (1996), Peters proposed to set \( h_a \) to \( \alpha^{-1} \) and \( h_{mn} \), respectively. Iden and Durner (2014) adopted this approach in their revised PDI model. For bimodal models (Durner, 1994; Romano et al., 2011) one can easily set \( h_a \) to \( \min(\alpha_1^{-1}, \alpha_2^{-1}) \) and \( \min(h_{mn1}, h_{mn2}) \), respectively (Peters & Durner, 2015; Weber et al., 2017). Therefore, the parameter \( h_a \) should not be viewed as an “extra parameter” as it was stated by W19. The same holds for the smoothing parameter \( b \) in the function for \( S_{nc} \) proposed by Iden and Durner (2014) because it also depends on the parameters of the capillary saturation function and therefore can be calculated from the other model parameters. For details we refer to the original publications. The reason to introduce \( h_a \) was to give the function \( S_{nc} \) the desired shape, that is, a linear decrease with \( x \) in the dry range and a constant value for high capillary saturations. Summing up, the number of adjustable (“free”) parameters of the PDI and W19 models is the same.

### 1.2. Shape of the Noncapillary Saturation Function

The new formulation for \( S_{nc} \) proposed by W19 is indeed innovative, deserves further consideration, and a critical analysis. The requirements for \( S_{nc} \) are summarized by W19 as follows:

(i) continuous differentiability over the entire suction range,

(ii) value of unity close to the air entry suction and a slower decrease than the capillary saturation function \( S_c \) on the wet end of the WRC to prevent an undesired multimodality in the water capacity function,

(iii) linear decrease to 0 on the dry end if plotted versus \( x \), and

(iv) achieving (i–iii) without introducing an extra model parameter.

As discussed above, the last requirement is met by PDI and W19. The remaining three requirements are all fulfilled by the PDI and requirement (i) and (ii) are also fulfilled by W19. However, requirement (iii) is only partially fulfilled by W19. Before we discuss this in detail, we want to briefly review the rationale for this premise. Experimental evidence has shown a linear decrease of water content with \( x \) at high suctions for a large set of measurements since the publication of Campbell and Shiozawa (1992). However, theoretical considerations (e.g. Tuller & Or, 2005) propose a convex shape of \( S_{nc}(x) \). Physically, this implies that the decrease in water content becomes smaller with increasing \( x \). The data of the silt loam from Schelle et al. (2013), shown Figure 7b in W19, for example, indicate that the WRC is slightly convex in the dry range. Therefore, requirement (iii) could be reformulated to “linear or convex decrease to 0 on the dry end if plotted versus \( x \)”.

We note at this point that the original PDI formulation fulfills requirement (iii) but is not in agreement with the theory of Tuller and Or (2005).

The function \( S_{nc}(x) \) in the W19 model is only linear at suctions beyond which the capillary saturation function approaches zero and remains constant. The reason for this is that the integral \( \left[ S_c(\bar{x}) - 1 \right] d\bar{x} \)
Figure 1. Illustration of the water retention model by W19 for different pore-size distributions. Left: Capillary retention functions, center: Results of integrating $S_{\text{c}}$ w.r.t. $x$ (Equation 4 of W19, $S_{\text{nc}}$), right: resulting noncapillary saturation functions $S_{\text{nc}}$. The van Genuchten parameter $n$ of the capillary saturation function was varied and $\alpha$ was 0.01 cm$^{-1}$ in all cases. The numerical integration to compute $S_{\text{nc}}^\Delta$ was performed with the trapezoidal rule and $\Delta x = 0.01$.

(Equation 4 in W19), where $\bar{x}$ is a dummy variable of integration which represents $x$, becomes linear beyond that suction. For capillary saturation functions representing narrow pore-size distributions (large values of van Genuchten $n$ or small value of Kosugi $\sigma$), the desired linear shape of $S_{\text{nc}}(x)$ in the relevant range of suction is warranted. However, for soils with wide pore-size distributions (small $n$, large $\sigma$), this linearity occurs only at suctions very close to oven dryness (see Figure 3 in W19). In these cases, the $S_{\text{nc}}(x)$ of W19 is concave and therefore in contradiction to requirement (iii) formulated in W19. This becomes evident in Figure 7b in W19 in which $S_{\text{nc}}(x)$ is concave because of the relatively wide pore-size distribution of the silt loam. We note that W19 acknowledge that their function is “close to linear in the high pF range” (caption to Figure 3 in W19), but unfortunately W19 do not analyze the consequences. We emphasize that the mechanisms of capillary water retention and water adsorption are not related (Lebeau & Konrad, 2010). Despite this, the W19 model uses the shape of the capillary saturation function to derive the shape of the noncapillary saturation function. Obviously, the connection between these two unrelated physical phenomena is too strong in the W19 model. Figure 1 shows this behavior for a wide range of capillary saturation functions. Requirement (iii) is here strictly fulfilled only for sandy soils with rather narrow pore-size distributions. This has direct implications for the predicted film conductivity function as will be shown below.

Hydraulic functions are mathematical formulations used to represent the overall hydraulic properties effectively, that is, total water contents and liquid hydraulic conductivities as functions of suction. Therefore, the subfunctions (e.g., $S_{\text{c}}(x)$ and $S_{\text{nc}}(x)$), and especially their parameters, should not be interpreted in a strict physical sense. However, their shapes should describe the macroscopic phenomena, which in turn represent microscale physical properties, as closely as possible within the limited complexity of the models. One could, for example, argue that in case of fitting the whole water retention function to data available in the complete moisture range, the physically incorrect concave shape of $S_{\text{nc}}(x)$ might be compensated by an increased convexity in $S_{\text{c}}(x)$. This will, however, (i) decrease flexibility of the function $S_{\text{c}}(x)$, and (ii) decrease the accuracy for predicting hydraulic conductivity. Regarding (i), the flexibility in $S_{\text{c}}(x)$ might decrease because the parameters for the capillary part have to be adjusted not only to describe $S_{\text{c}}(x)$ but also to compensate for the undesired concave shape in $S_{\text{nc}}(x)$. Regarding (ii), the accuracy of the conductivity prediction might decrease because $S_{\text{c}}(x)$ and $S_{\text{nc}}(x)$ affect the shapes of the capillary and film conductivities, respectively.

Hence, altering the shape of $S_{\text{c}}(x)$ to compensate for the structurally wrong $S_{\text{nc}}(x)$ leads to an altered shape of the capillary conductivity function predicted by the capillary bundle model (e.g., Mualem, 1976).

1.3. Non-Capillary Conductivity

W19 directly incorporate their $S_{\text{nc}}$ function into the noncapillary conductivity model of Peters (2013), replace the parameter $h_2$ by $h_2 = 1$ cm and claim that this formulation is in agreement with the theoretical model of Tokunaga (2009). This is incorrect. In his seminal paper, Tokunaga (2009) derived the film
conductivity w.r.t. suction under certain assumptions and simplifications for packings of monodisperse grains. His model is based on the relationship of film thickness and Gibbs free energy represented by suction (as derived by Langmuir, 1938) and the solution of the Navier-Stokes equations for unit-gradient flux in these films. Peters (2013) adopted this model by omitting all constants while sustaining the slope of $a = -1.5$ in the double-log plot of noncapillary conductivity $K_{nc}$ (L/T) versus suction in the dry range, and applied it to real data. We note that different mechanisms are responsible for noncapillary liquid conductivity, namely the conductivity due to water flow in thin and thick films, corners and edges (Tuller & Or, 2001). Here, we use the notation “noncapillary conductivity” although the theory of Tokunaga (2009), which was simplified by Peters (2013) and then used in the PDI, accounts only for conductivity in liquid films. This formulation for relative noncapillary conductivity ($K_{nc,r}$) is simply:

$$K_{nc,r}(h) = \begin{cases} 1 & \text{if } h \leq h_s \\ \left(\frac{h}{h_s}\right)^{-a} & \text{if } h > h_s \end{cases}$$

(1)

Peters (2013) used his formulation of $S_{nc}$ (Equation 3 in Peters, 2013), applied some simplifications, substituted $h$ in Equation 1 by $h(S_{nc})$, and finally derived:

$$K_{nc,r}(S_{nc}) = \left(\frac{h_0}{h_s}\right)^{a(1-S_{nc})}$$

(2)

We note that mathematically, Equation 2 is only valid for Equation 3 in Peters (2013). Due to the very similar shape of the $S_{nc}$ function of Iden and Durner (2014) for $h \gg h_v$, the PDI model has the correct shape of the noncapillary conductivity, which is in agreement with Tokunaga (2009) and Peters (2013).

In contrast, the formulation of W19 reads:

$$K_{nc,r}(S_{nc}) = \left(\frac{h_0}{h_v}\right)^{a(1-S_{nc})}$$

(3)

In which $h_v$ is unity in the case that $h$ is given in cm (W19). Obviously, the derivatives of Equations 2 and 3 with respect to $S_{nc}$ are given by $-a \log(h_0 / h_v)$ for the PDI (Peters, 2013) and $-a \log(h_0)$ for the W19 model. Even if $S_{nc}$ does decrease linearly with $x$, there is a clear difference between the slopes of $K_{nc,r}$ with respect to $S_{nc}$ between the PDI and the W19 model.

As shown in Figure 1, the slope of $S_{nc}(x)$ as suggested by W19 is linear only for rather narrow pore-size distributions. We start the analysis with the simple case in which $S_{nc}(x)$ is linear (large $n$) and show the consequences of using the W19 function to predict $K_{nc,r}$ by Equation 3 in Figure 2. Depending on the value of the van Genuchten parameter $\alpha$, the slope of $K_{nc,r}(x)$ can differ greatly from $-1.5$, the value derived by

Figure 2. Dependence of $K_{nc,r}(x)$ on the van Genuchten parameter $\alpha$ for soils with a narrow pore-size distribution ($n = 3$). Left: Capillary saturation function, center: corresponding noncapillary saturation functions, right: resulting relative noncapillary conductivities using Equation 3 “W19” Dashed lines in right plot: relative noncapillary conductivity if $h_v$ is substituted by $h_v = \alpha^{-1}$ in Equations 3 “W19 ($h_v = \alpha^{-1}$)”.

Tokunaga (2009). The only case where the slope is correct is for \( \alpha^{-1} r_1 \approx 1 \) cm. However, there is almost no natural soil with such a high value of \( \alpha \). Figure 2c shows that the W19 model always overestimates the slope of \( n_c, r(K_x) \). For the cases shown, the slopes vary from \( \approx -1.8 \) (for \( \alpha^{-1} r_1 = 10.1 \) cm) to \( \approx -3.8 \) (for \( \alpha^{-1} r_1 = 4110 \) cm). Thus, the predicted noncapillary conductivity decreases more rapidly with increasing suction for fine-textured soils than for coarse-textured soils. The dashed lines in Figure 2 show the results of Equation 3 if we substitute \( r_1 h \) with \( \alpha^{-1} a h \). Obviously, replacing \( r_1 h \) by \( \alpha^{-1} a h \) leads to the slope of \( -1.5 \) as derived by Tokunaga (2009). However, the reintroduction of \( a h \) eliminates the claimed advantage of W19 over the formulation of Iden and Durner (2014), that is the nonnecessity of the parameter \( a h \). The analysis in Figure 2 uses a narrow pore-size distribution with a van Genuchten parameter \( n = 3 \) and does therefore only treat cases in which \( S_{nc}(x) \) of W19 is indeed linear.

Figure 3 shows the shape of the \( K_{nc,m}(x) \) function for soils with wider pore-size distributions (smaller values of \( n \)). In this case, the function \( S_{nc}(x) \) is not linear (Figure 1). The slope of \( \log_{10} K_{nc,m}(x) \) for the W19 formulation (Equation 3) depends strongly on \( x \), the function is nonlinear, and this contradicts Tokunaga (2009) again. This undesired behavior of the W19 model becomes evident in the conductivity plots of soils d, I, and m in Figure 6 of W19.

There seems to be no straightforward way to transform the shape of \( K_{nc,m}(x) \) of W19 to the shape predicted by Tokunaga’s model. We conclude that the W19 film-conductivity formulation is not in agreement with the model of Tokunaga. If, despite the violation of the linearity requirement, the \( S_{nc} \) formulation of W19 is used for soils with wide pore-size distributions, we suggest to decouple the \( S_{nc} \) and \( K_{nc,m} \) again and directly formulate \( K_{nc,m} \) as function of suction, using Equation 2 (Equation 16 in Peters [2013]).

2. Concluding Remarks

W19 proposed a new function for noncapillary water retention in variably saturated porous media, which is closely related to the shape of the capillary retention function. This new function was implemented into the PDI model system. For soils with narrow pore-size distributions, the W19 noncapillary saturation function decreases linearly to 0 on the dry end if plotted versus \( x \). However, for soils with wide pore size distributions, the shape of \( S_{nc}(x) \) is no longer linear but concave. This contradicts the linearity requirement stated in W19 and theoretical considerations. If the W19 \( S_{nc}(x) \) function is integrated into a simplified version of the noncapillary conductivity model of Peters (2013) as suggested by W19, it does not yield a slope of \(-1.5\) in the double-log conductivity versus pF plot. In fact, the slope depends on the shape of \( S_{nc}(x) \) and, due to their close relation in W19, on the shape of the capillary saturation function \( S_c(x) \). Therefore, the W19 model is
not, opposed to what is stated by the authors, in agreement with the theory of Tokunaga (2009). We note at this point that the slope in Tokunaga (2009) was derived for packings of monodisperse smooth grains and might not strictly be applicable to real soils consisting of polydisperse grains with differing surface properties. An in-depth discussion of these issues is, however, beyond the scope of this comment.

We suggest to use the W19 model for \( S_{nc}(x) \) very cautiously and only for soils with narrow pore-size distributions. For such soils, replacing \( h_f \) by \( h_i \) in the film conductivity function is a remedy, if the model shall be in agreement with the model of Tokunaga (2009). Unfortunately, this makes the model structurally even more similar to the original PDI. For soils with wide pore-size distributions, there seems to be no simple solution for the problems illustrated in this comment. If the W19 formulation is used for any soil, one should be aware that it might be able to describe the data but that it is neither in agreement with the linearity requirement for water retention in dry soil, nor with the theory of Tokunaga (2009).

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