A Simple Model to Predict Hydraulic Conductivity in Medium to Dry Soil From the Water Retention Curve

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Abstract The mathematical representation of the soil hydraulic properties is of central importance for modeling water, solute and energy transport in soils. The established models of the water retention and hydraulic conductivity curves account for capillary water retention and conductivity, but neglect water adsorption and water flow in films and pore corners. They are therefore suited for modeling flow and transport processes in the medium to wet moisture range, but are susceptible to failure in dry soil. The model system developed by Peters (2013, https://doi.org/10.1002/wrcr.20548; 2014, https://doi.org/10.1002/2014wr016107) and Iden and Durner (2014, https://doi.org/10.1002/2014wr015937) (PDI in the following) is a simple parametric framework that overcomes these structural shortcomings. However, it requires one additional parameter to scale the hydraulic conductivity curve in the moisture range where non-capillary flow dominates. Measured conductivity data are required to determine this scaling parameter and to compute the hydraulic conductivity over the complete moisture range. In this contribution, we first show that the original PDI model is in close agreement with a comprehensive model for film conductivity in porous media. We then derive a physically-based approach to predict the film conductivity from the water retention curve. This improved PDI model has the same number of parameters as established models and provides a complete prediction of the hydraulic conductivity curve including non-capillary flow if water retention data and the saturated conductivity are known. Application to literature data covering a broad range of textures shows an improvement of the conductivity prediction by the factor five if compared to the van Genuchten/Mualem model.

1. Introduction

In order to adequately model water, solute and energy transport in the vadose zone, an accurate mathematical representation of the soil hydraulic properties, that is, the soil water retention and hydraulic conductivity curves, is required. Common representations of both functions, as given, for example, by van Genuchten (1980), Durner (1994), or Kosugi (1996), describe capillary water retention and conductivity, but neglect water adsorption, film and corner flow. Therefore, they are well suited to model transport processes in the medium to wet moisture range. They fail, however, to describe water transport when the soil becomes dry (Peters et al., 2015).

Most traditional water retention functions assume a distinct residual water content, which is asymptotically reached at high suctions. This residual water content is either interpreted as water that is held by adsorptive forces (Corey & Brooks, 1999) or it is used as a mere fitting parameter. Thirty years ago, Nimmo (1991) discussed the problem and the fundamental misconception of this approach. From a physical point of view, the water film thickness will continually decrease as suction increases (Tuller & Or, 2005) and finally the water content becomes by definition zero at oven dryness (Schneider & Goss, 2012). To our knowledge, Campbell and Shiozawa (1992) were the first to show that in the hygroscopic moisture range, the water content often decreases linearly toward zero if it is plotted versus the log of suction. This was accounted for in the retention models of Rossi and Nimmo (1994), Fayer and Simmons (1995) and Khlosi et al. (2006). The frequently used functions of Fayer and Simmons (1995) and Khlosi et al. (2006) (e.g., Lebeau & Konrad, 2010) do not predict a water content of zero at oven dryness for soils with wide pore-size distributions (Peters et al., 2013). Moreover, these models sometimes predict even an increase in water content with increasing suction near saturation, which is physically wrong (Peters et al., 2011). Therefore, Peters (2013) suggested an alternative model formulation, which describes water retention by a linear superposition of the capillary and non-capillary components. This model was improved by Iden and Durner (2014).
The established models for hydraulic conductivity, for example, Mualem (1976), account only for capillary flow and neglect all non-capillary flow processes. However, water in films on solid surfaces and in corners contribute also to hydraulic conductivity, which becomes more and more important in the medium to dry moisture range. This was accounted for in the hydraulic conductivity models by Tuller and Or (2001), Peters and Durner (2008), Lebeau and Konrad (2010), Zhang (2011) and Peters (2013). The model of Tuller and Or (2001) is theoretically demanding, and due to its complexity and its coupling with a rather inflexible retention function (Lebeau & Konrad, 2010), it is seldom used in applied studies or numerical codes. The film conductivity model of Lebeau and Konrad (2010), in the following abbreviated with LK, is easier to implement and, due to its strong physical basis, represents a benchmark to evaluate more simplified approaches. In contrast to the model of Tokunaga (2009), also used by Zhang (2011) and Peters (2013), the LK model does not only account for the ionic-electrostatic compound, but also for the molecular compound of the disjoining pressure isotherm, which is used to describe film thickness as function of suction. The ionic-electrostatic forces are dominant in holding the liquid water in films at a distance >10 nm from the grain surface, whereas the molecular (van der Waals) forces are dominant in thin films (<10 nm). In addition, based on the work of Or and Tuller (2000), the LK model accounts for increasing viscosity near the mineral surfaces. Modaresi Rad et al. (2020) implemented it into their hydraulic conductivity model. In applied studies, however, the LK model is seldom used.

We note that the mechanisms causing non-capillary water retention and conductivity are manifold, and include water adsorption and conductivity due to water in thin and thick films, corners and edges of the complex pore space (Tuller & Or, 2001). The models which account for non-capillary mechanisms are, however, often simplified and should only be regarded as effective descriptions. In the following, we will not differentiate the many causes linguistically, and use the terms non-capillary conductivity and film conductivity synonymously, depending on the sources referred to.

The structure of the water retention models suggested by Peters (2013) and Iden and Durner (2014), and the related formulations for the capillary, non-capillary, and total hydraulic conductivity (Peters, 2013, 2014) is referred to as PDI model system by the authors. The non-capillary conductivity in the PDI model is based on the film conductivity model of Tokunaga (2009) and therefore it neglects both the molecular component of the disjoining pressure isotherm and the increased viscosity near mineral surfaces, which become important in thin films, that is, at dry conditions. Nevertheless, it is used to describe effectively the complete conductivity in the medium to dry moisture range.

Comparisons with data covering a large variety of soils showed that the PDI model system can describe the water retention and hydraulic conductivity over the full moisture range well, despite its simplification of the underlying processes (Iden et al., 2021; Peters, 2013; Rudiyanto et al., 2015; Weber et al., 2017). Due to its simple formulation, it can easily be used in parameter estimation and numerical simulation studies for variably-saturated water flow (Luo et al., 2020). A distinct disadvantage of the PDI model system is that the film conductivity is only expressed as a relative conductivity function, which must be scaled by a factor to contribute to the total liquid conductivity function. This means that suitable experimental data, that is, unsaturated conductivity data in the medium to dry moisture range, are required to quantify the film conductivity component. Therefore, it is not possible to predict the hydraulic conductivity curve from the water retention characteristics and saturated conductivity alone. This is in contrast to the established model formulations, for example, van Genuchten/Mualem (Mualem, 1976; van Genuchten, 1980), or to the LK model, and reduces the practical applicability, since the required conductivity data are often not available. The widely used simplified evaporation method (Peters & Durner, 2008; Schindler, 1980), for example, yields unsaturated conductivity data in the suction head range between ~1 and 10 m, in which sandy soils show a transition from capillary-dominated water flow toward a flow regime that is dominated by non-capillary flow mechanisms. Unfortunately, fine textured soils exhibit this transition zone usually at suctions larger than 10 m. Therefore, the PDI models can be easily applied to the data of sandy soils but not to the data of fine textured soils because the required information for the scaling parameter of the non-capillary conductivity model is missing.

Summarizing, we identified a theoretical and a practical shortcoming of the PDI non-capillary conductivity function. The theoretical shortcoming is the negligence of two physical processes, which become important under very dry conditions when very thin water films prevail. The practical shortcoming is the need of an
extra free parameter that is not easily obtained from measurements. Since the LK model is physically based and can be used to predict film conductivity, it can serve as a benchmark to analyze the adequacy of the simple PDI model and provides a basis to derive a prediction scheme, which removes the fitting parameter in the PDI.

The aim of this study is therefore (a) to analyze the simple PDI model of relative film conductivity by comparing it with the comprehensive physically-based model of LK, and (b) to propose a simple but physically based prediction of the film conductivity within the PDI model system.

2. Theory

In this section, we begin with a concise review of the mathematical formulation of the PDI model, which is the starting point for its improvement later in this paper. Second, we assess and justify the simplifications of the PDI model for relative non-capillary conductivity based on the LK model. Finally, we propose an PDI formulation where non-capillary conductivity is predicted from the water retention data.

2.1. PDI Model System

2.1.1. PDI Water Retention Function

The superposition of a capillary saturation function $s_c$ and a non-capillary saturation function $s_{nc}$ is expressed as (Iden & Durner, 2014):

$$\theta(h) = \left( \theta_s - \theta_r \right) s_c + \theta_r s_{nc}. \quad (1)$$

The first right term considers water stored in capillaries, while the second term refers to the storage of water in adsorbed films and pore corners. $\theta$ (m$^3$ m$^{-3}$) is the total water content, $h$ (m) is the suction head and $\theta_s$ (m$^3$ m$^{-3}$) and $\theta_r$ (m$^3$ m$^{-3}$) are the saturated and maximum adsorbed water contents. To meet the physical requirement that the capillary saturation function reaches zero at oven dryness, a basic saturation function $\Gamma(h)$ is scaled by (Iden & Durner, 2014):

$$\Gamma(h) = \Gamma(0) - \Gamma(h_0) \frac{1 - \Gamma(h_0)}{1 - \Gamma(0)}, \quad (2)$$

with $h_0$ (m) being the suction head at oven dryness, which can be set at $10^{-18}$ m (Schneider & Goss, 2012). $\Gamma(h)$ can be any uni- or multimodal saturation function, for example, the unimodal functions of van Genuchten (1980), Kosugi (1996), or their bimodal versions (Durner, 1994; Romano et al., 2011). In this study, we use the constrained unimodal saturation function of van Genuchten (1980):

$$\Gamma(h) = \left( \frac{1}{1 + \alpha h^n} \right)^m, \quad (3)$$

where $\alpha$ (m$^{-1}$) and $n$ (–) are shape parameters and $m = 1 - 1/n$.

The saturation function for non-capillary water (Figure 1, dash-dotted line) is given by a smoothed piecewise linear function (Iden & Durner, 2014), which is here rewritten, yielding:

$$s_{nc}(h) = \ln\left( h / h_0 \right) - b \ln\left( 1 + \left[ h / h_0 \right]^{1/b} \right) / \ln(h_0 / h_0). \quad (4)$$

The parameter $h_0$ (m) reflects the suction head where non-capillary water reaches its saturation and is set to $a^{-1}$ (Peters, 2013). The parameter $h_0$ is the suction head where the water content reaches zero and this reflects the suction at oven dry conditions. $s_{nc}(h)$ increases linearly from zero at oven dryness to its maximum.
value 1 at \( h_0 \) and then remains constant toward saturation. In order to ensure a continuously differentiable water capacity function, it must be smoothed around \( h_0 \), which is achieved by the smoothing parameter \( b \) (Iden & Durner, 2014), which is here given by:

\[
b = b_0 \left( 1 + 2 \frac{1 - e^{-h}}{n^2} \right),
\]

where \( b_0 = 0.1 \ln(10) \) and \( b_1 = \left( \theta_s / (\theta_s - \theta_f) \right)^2 \).

2.1.2. PDI Hydraulic Conductivity Model

The hydraulic conductivity model is expressed as (Peters, 2013):

\[
K = K_c + K_{nc} + K_v = K_{s,c} K_{r,c} \left( S_c \right) + K_{s,nc} K_{r,nc} \left( S_{nc} \right) + K_v,
\]

where \( K_{r,c} \) and \( K_{r,nc} \) are relative conductivities for the capillary and non-capillary components, \( K_{s,c} \) (m s\(^{-1}\)) and \( K_{s,nc} \) (m s\(^{-1}\)) are the saturated conductivities for the capillary and non-capillary components, and \( K_v \) (m s\(^{-1}\)) is the isothermal vapor conductivity. Please see Saito et al. (2006) or Peters (2013) for details regarding the formulation of \( K_v \) as function of the water retention curve. The saturated conductivities for the capillary and non-capillary components can be expressed as \( K_{s,c} = (1 - \omega) K_s \) and \( K_{s,nc} = \omega K_s \), with \( K_s \) (m s\(^{-1}\)) being the saturated conductivity and \( \omega \) being a weighing parameter partitioning liquid conductivity between capillary and non-capillary components, constrained by \( 0 \leq \omega \leq 1 \). Note that both components of liquid conductivity are formulated as relative conductivities, which have to be scaled, whereas isothermal vapor conductivity is formulated as absolute conductivity.

Relative conductivity for water flow in capillaries is in this paper described by the pore bundle model of Mualem (1976a), which reads in the notation of Equation 2 (Peters, 2014):

\[
K_{r,c} \left( S_c \right) = \left( S_c \right)^2 \left( \frac{\tau}{\int_{-\infty}^{h_1} h^{-1} dX} \right)^2,
\]

where \( \tau \) is the tortuosity and connectivity parameter, and \( X \) is a dummy variable of integration. With the van Genuchten shape function for the capillary water retention, Equation 3, the analytical solution for Equation 7 is (Peters, 2014):
According to Tokunaga (2009), the decrease of film conductivity on the log-log scale should have a slope of −1.5. This holds for relative thick films (>10 nm), where the molecular component of the disjoining pressure and variation of viscosity near mineral surfaces can be neglected (Lebeau & Konrad, 2010). Peters (2013) adopted this relationship and expressed relative non-capillary conductivity function by:

\[
K_{r,nc} = \left( \frac{S_c}{S_{nc}} \right)^{1.5} \left( 1 - \frac{h^{1/m}}{1^{1/m}} \right)^m.
\]  

(8)

If the non-capillary saturation function is linear on the semi-log scale and starts to decrease at \( h_a \), the saturation-dependence of the non-capillary conductivity can be simply expressed as (Peters, 2013):

\[
K_{r,nc} = \begin{cases} 
\left( \frac{h_a}{h} \right)^{-1.5} & \text{for } h > h_a, \\
1 & \text{for } h \leq h_a.
\end{cases}
\]  

(9)

Compared to the established approaches, which neglect non-capillary water, the PDI formulation requires the additional parameter \( K_{r,nc} \) to calculate the hydraulic conductivity function.

### 2.2. Analyzing and Improving the PDI Formulation

#### 2.2.1. Comparison of the PDI Formulation With the Lebeau and Konrad Formulation

Appendix A.1 gives a brief overview of the Lebeau and Konrad (2010) film conductivity model, which accounts for the ionic-electrostatic (Equation A1) and the molecular compound (Equation A2) of the disjoining pressure isotherm. Both are used to describe film thickness as function of suction. Furthermore, LK accounts for increasing viscosity near the mineral surfaces (Equations A5 and A6). The film conductivity is given by Equation A4 for \( \delta > 10 \) nm and by Equation A5 for \( \delta < 10 \) nm. Since for large \( \delta \) (>10 nm), Equation A5 converges to Equation A4, we use Equation A5 for comparing the PDI non-capillary conductivity function with the LK model.

For comparison, we show in Figure 2 the relative conductivity curves of the PDI model (Equation 9) and the LK model (Equation A5), normalized to a value of 1 at a suction head of 0.1 m. The physical constants used in this study are the same as used by LK and given in Table A1. Remarkably both curves, the PDI model (Equation 9, black line) and the physically-based LK model (Equation A5, red line), are very similar over almost the entire relevant suction head range although the molecular component of disjoining pressure and increasing viscosity near the solid surfaces are neglected in the PDI. This at first unexpected result is explained by an almost perfect counter-balancing of the errors caused by the neglect of both effects. Neglect of the molecular component decreases the film thickness and therefore decreases hydraulic conductivity at a given suction head, whereas the neglect of the viscosity increase leads to an increase in film conductivity. The solid blue line in Figure 2 shows the case where the molecular component of disjoining pressure is considered, but not the variable viscosity. The dashed blue line shows the case where the variable viscosity is taken into account but not so the molecular pressure component. Incorporating both leads to the red line, which is the full LK model. Given the uncertainty range caused by the variability of the Hamaker constant (gray shaded area), we regard the simplifying assumptions of the Peters (2013) film conductivity model as justified from a practical point of view. We varied the temperature from 10°C to 30°C and found that the impact of temperature on the relative course of the LK model is negligible (not shown).
2.2.2. Calculation of Absolute Non-Capillary Conductivity From the Water Retention Curve

As stated above, the PDI model scheme requires the additional adjustable parameter $K_{s,nc}$ to scale the relative non-capillary conductivity function $K_{r,nc}$ to absolute non-capillary conductivity. We see no straightforward way to derive this scaling parameter directly from the parameters of the soil water retention curve. However, the retention function in the dry moisture region contains information about the specific surface area of the minerals (Tuller & Or, 2005) and hence implicitly about the effective particle diameter and film conductivity (Lebeau & Konrad, 2010).

Solving the Langmuir model for water adsorption (Equation A2) for film thickness and expressing the disjoining pressure $\Pi$ by the suction head $h$ yields:

$$
\delta = \frac{\pi k_b T}{eZ} \left( \frac{\varepsilon_r \varepsilon_0}{2} \right) \left( \rho g h \right)^{-0.5},
$$  \hspace{1cm} (11)

where $\varepsilon_r$ (-) and $\varepsilon_0$ ($C^2 \cdot T^{-1} \cdot m^{-1}$) are the static relative permittivity of the liquid phase and the permittivity of free space, respectively, $k_b$ ($J \cdot K^{-1}$) is the Boltzmann constant, $T$ (K) is the absolute temperature, $e$ ($C$) is the electron charge, $Z$ is (-) the valence, $\rho$ ($kg \cdot m^{-3}$) is the liquid density and $g$ ($m \cdot s^{-2}$) is the gravitational acceleration constant. For packings of monodisperse spheres and constant viscosity, Tokunaga (2009) found the following relationship between non-capillary conductivity and film thickness:

$$
K_{s,nc} = \frac{\rho g}{\pi \eta D} (1 - \varphi) 4 \delta^3.
$$  \hspace{1cm} (12)

where $\varphi$ (-) is porosity and $D$ (m) is the grain diameter. Substituting Equation 11 into Equation 12 (i.e., considering only the ionic-electrostatic component of disjoining pressure and neglecting increased viscosity near mineral surfaces), and using an effective grain diameter $D_e$ (m) yields a simplified version of the Tokunaga (2009) model:

$$
K_{s,nc}(h) = E h^{-1.5},
$$  \hspace{1cm} (13)

with

$$
E = \frac{4 \pi^2 \rho g (1 - \varphi)}{\eta D_e} \left( \frac{\varepsilon_r \varepsilon_0}{2} \right)^{1.5} \left( \frac{k_b T}{eZ} \right)^{1.5} \left( \rho g \right)^{1.5}.
$$  \hspace{1cm} (14)

$E$ equals the absolute film conductivity in $m^{5/2} \cdot s^{-1}$ at $h = 1$ m. Based on the work of Tuller and Or (2005), LK derived the equivalent grain diameter from the water content $\theta_m$ at $h_m = 1,000$ m, where capillary forces can be neglected:

$$
D_e = 6(1 - \varphi) \left( \frac{A_H}{6 \pi \eta \varphi g h_m} \right)^{1/3} \frac{1}{\theta_m},
$$  \hspace{1cm} (15)

where $A_H$ [J] is the Hamaker constant (see Appendix A). Combining Equations 13–15 yields:

$$
K_{s,nc}(h) = c \theta_m h^{-1.5},
$$  \hspace{1cm} (16)

where the constant $c$ is defined as

$$
c = \frac{2}{3} \frac{\pi^{7/3}}{\eta (\rho g)^{1/6}} \left( \frac{6}{A_H} \right)^{1/3} \left( \frac{\varepsilon_r \varepsilon_0}{2} \right)^{3/2} \left( \frac{k_b T}{eZ} \right)^{3/2} h_m^{1/3}.
$$  \hspace{1cm} (17)

Note, that $\varphi$ is eliminated and has therefore not to be specified. For the values listed in Table A1 and setting $h_m = 1,000$ m as proposed above, $c = 1.35 \times 10^{-8} \cdot m^{5/2} \cdot s^{-1}$ or, if suction head is expressed in cm and time in d, $c = 98 \text{ cm}^{5/2} \cdot \text{d}^{-1}$. 

In essence, this approach is very similar to the predictive conductivity model of LK, except that we neglect the molecular components of the disjoining pressure and increasing viscosity near mineral surfaces. As discussed in the context of Figure 2, we think that these simplifications are justified due to the counter-balancing of both simplification errors, and therefore arrive at a fairly simple formulation.

### 2.2.3. Re-Formulation of Non-Capillary Conductivity Within the PDI Model System

The prediction scheme for non-capillary conductivity given in Equation 16 is only valid above a critical suction (Tokunaga, 2009). Therefore, we may combine it with the PDI model (Equation 9). Since non-capillary conductivity is only relevant for \( h \gg h_u \), we focus on the linearly decreasing part of \( K_{nc}(h) \) of Equation 9. Multiplication with the saturated non-capillary conductivity \( K_{s,nc} \) yields the non-capillary conductivity function in the range \( h \gg h_u \):

\[
K_{nc}^*(h) = K_{s,nc} \left( \frac{h}{h_u} \right)^{-1.5},
\]

which is similar to Equation 16 with

\[
c\theta_m = \frac{K_{s,nc}}{h_u^{-1.5}},
\]

leading to:

\[
K_{s,nc} = h_u^{-1.5} c\theta_m,
\]

with this we have arrived at a direct prediction of the non-capillary conductivity from the water retention curve. Combining Equation 10 and Equation 20 yields

\[
K_{nc} = c \theta_m h_u^{-1.5} \left( \frac{h_0}{h_u} \right)^{-1.5(1-S_{nc})},
\]

and the equation for the entire hydraulic conductivity curve becomes:

\[
K(h) = K_{s,e} K_{r,e} \left( h \right) + K_{nc}(h) + K_c(h).
\]

Compared the original PDI model the number of adjustable parameters is decreased by one because \( c \) is given by Equation 17. This means that the number of estimated/adjusted parameters of the improved PDI model is now equal to that of established models which do not include non-capillary mechanisms of storage and flow, for example, the van Genuchten/Mualem model. In the new PDI, both the non-capillary conductivity and the isothermal vapor conductivity are predicted in absolute terms and only the relative capillary conductivity must be scaled with the saturated capillary conductivity. We note that the value of the constant \( c \) is based on several simplifications. If conductivity data are available in the moisture range where non-capillary mechanisms dominate, it is possible to adjust parameter \( c \) to achieve a data-fitted description of the conductivity curve.

### 3. Material and Methods

#### 3.1. Data for Model Testing

To test our approach with special focus on the conductivity prediction in the higher suction head range, we applied the improved PDI model to the same data sets which were used by Peters (2013) for testing the original PDI model. An overview with reference to the data sources is given in Table 1. For further details on the methods used for data acquisition we refer to Peters (2013) and the original study.
3.2. Model Comparison

The PDI model with the van Genuchten saturation function and the new prediction scheme for the non-capillary conductivity is defined by Equations 1–5 for the retention curve and by Equations 8, 21, 22 for the conductivity curve. To assess its performance, we compared it with the original van Genuchten/Mualem model, which was extended by the isothermal vapor conductivity to make the comparison fair and reasonable. Both models were fitted in two different modes. In the first mode, all retention and conductivity parameters were optimized. This is common practice when experimentally measured data are available. The parameter $\tau$ was allowed to vary within limits of physical consistency according to Peters et al. (2011) and Peters (2014). In particular, for the van Genuchten/Mualem model (VGM*6), this increases the flexibility to match observed conductivity data considerably. If the scaling parameter $c$ for non-capillary conductivity is included in the list of free parameters, the PDI model (model PDI*7) has one parameter more than the classic VGM. With $c = 1.35 \times 10^{-8}$ m$^{5/2}$ s$^{-1}$, corresponding to $h_m = 1,000$ m (PDI*6), the number of free parameters is equal for VGM and PDI (see Table 2).

In a second mode, we compared the two model approaches for a situation, where no unsaturated conductivity data are available. Now, the whole conductivity function is predicted from the retention function plus a measured (or assumed) value of $s_K$. In this case, only retention curve parameters are estimated and the respective number of free model parameters are identical for VGM and PDI (four in both cases). We indicate these model modes by VGM*4 and PDI*4.

The parameter estimation was done as described in Peters (2013). The five model settings (Table 2) were fitted to the data by minimizing the sum of weighted squared residuals between modeled and measured water retention and log conductivity data:

$$\phi(b) = w_\theta \sum_{i=1}^{n_\theta} \left[ \theta_i - \theta_{\text{mod},i}(b) \right]^2 + w_K \sum_{i=1}^{n_K} \left[ \log_{10}(K_i) - \log_{10}(K_{\text{mod},i}(b)) \right]^2,$$

(23)

where $\theta_i$ and $\theta_{\text{mod},i}$ are the measured and modeled water contents, $K_i$ and $K_{\text{mod},i}$ are measured and modeled hydraulic conductivities, $n_\theta$ and $n_K$ are the respective number of data points, $w_\theta$ and $w_K$ are weights for the two data groups and $b$ is the parameter vector containing all adjustable parameters. According to Peters (2013), the weights $w_\theta$ and $w_K$ were set to 10,000 and 16, respectively. The shuffled-complex-evolution

Table 1

| Data set               | Reference                        | $K_i$ [m s$^{-1}$] |
|-----------------------|----------------------------------|--------------------|
| Minasny Sand          | Minasny and Field (2005)         | $1.16 \times 10^{-6}$* |
| Schindler Sand        | Schindler and Müller (2006)      | $1.16 \times 10^{-6}$* |
| Berlin Sand           | Peters (2013)                    | $1.16 \times 10^{-6}$* |
| Rehovot Sand          | Mualem (1976b)                   | $1.33 \times 10^{-4}$ |
| Gilat Loam            | Mualem (1976b)                   | $2.00 \times 10^{-6}$ |
| Pachapa Fine Sandy Clay (PFSC) | Mualem (1976b)               | $1.40 \times 10^{-6}$ |
| Minasny Loam          | Minasny and Field (2005)         | $1.16 \times 10^{-6}$* |
| Sandy Loam            | Pachepsky et al. (1984)          | $9.26 \times 10^{-7}$ |
| Silt Loam             | Pachepsky et al. (1984)          | $3.59 \times 10^{-7}$ |
| Clay Loam             | Pachepsky et al. (1984)          | $7.52 \times 10^{-8}$ |

Note. $s_K$ was kept constant at known values, if available. For Minasny Sand, Minasny Loam, Schindler Sand and Berlin Sand there were no $K_i$ values available. Therefore, reasonable values were assumed ($1.16 \times 10^{-4}$ m s$^{-1}$ or 1,000 cm d$^{-1}$ for the sands and $1.16 \times 10^{-5}$ m s$^{-1}$ or 10 cm d$^{-1}$ for the loam) and are indicated by the asterisk. These assumptions are in agreement with the parameters given by Carsel and Parrish (1988) for the respective texture classes. The sequence of the soils was chosen according to their pore-size distributions, starting with the soil with narrowest pore-size distribution.
Table 2
Adjustable Parameters for the Model Comparison

| Model     | No. of free parameters | Retention curve parameters | Conductivity curve parameters |
|-----------|------------------------|-----------------------------|------------------------------|
| VGM*6     | 6 (4 + 2)              | ✓                           | ✓                            |
| PDI*7     | 7 (4 + 3)              | ✓                           | ✓                            |
| PDI*6     | 6 (4 + 2)              | ✓                           | ✓                            |
| VGM*4     | 4 (4 + 0)              | ✓                           | ✓                            |
| PDI*4     | 4 (4 + 0)              | ✓                           | ✓                            |

Note. N: number of adjustable parameters, ✓: fitted parameter, Meas.: set to measured (or assumed) value as given in Table 1. ✓: set constant. If set constant, parameters \( \theta \) and \( c \) were 0.5 and \( 1.35 \times 10^{-8} \) m s \(^{-1} \), respectively.

As the number of estimated parameters varied, the performances of the models were compared using the Akaike Information Criterion corrected for small sample size, AIC\(_c\) (Akaike, 1974; Hurvich & Tsai, 1989). Table A2 in the appendix summarizes the AIC\(_c\) values. In the remainder of this article, the emphasis is on the comparison of models which have the same number of parameters, that is, VGM*6 versus PDI*6, VGM*4 versus PDI*4. Therefore, the AIC\(_c\) values are not discussed in detail in the main text.

4. Results and Discussions

4.1. Model Comparison

A comparison of all models for all data sets is shown in Figure 3. The van Genuchten-Mualem model adequately describes the data in the moist range, but is neither able to describe nor to predict the measured data in the medium to dry range. If all parameters are adjusted (model VGM*6), the better match of the model in the medium to dry range worsens the match in the wet moisture range, where capillary storage and conductivity dominate. This discrepancy is due to the structural inability of the VGM model to incorporate the effects of water in films and corners into the retention and conductivity functions. The pure prediction of unsaturated conductivity by model VGM*4 interestingly leads to an even better match of the conductivity data in the capillary-dominated range but to a complete mismatch in the drier range. Fitting the PDI model adjusting all parameters (model PDI*7) yields an almost perfect fit, as already demonstrated for a wide variety of soils in previous studies (e.g., Peters, 2013; Weber et al., 2017). It confirms the structural adequacy and the flexibility of the underlying functions. We note that the PDI*7 model has one free parameter more than the VGM*6.

The case PDI*6 is of particular interest, because it has high practical relevance. Today there exist more and more data bases with measured retention data in the full moisture range and conductivity data in the capillary dominated range, which are obtained by a combination of the simplified evaporation method (Peters & Durner, 2008b; Schindler, 1980) and the dew point method (Campbell et al., 2007). Thus, fitting PDI*6 is the typical case if these data are available. Figure 3 shows the striking difference of the fits of the PDI*6 model compared to the original VGM*6 model. In both cases the same parameters, namely the four retention parameters and \( K_s \) and \( r \), are fitted.

Finally, even the purely predicted unsaturated conductivity functions of the new model PDI*4 match the measured data in most cases well. Similar results were also found by Lebeau and Konrad (2010) for their model. The improvement of the PDI conductivity prediction as compared to the established VGM prediction is evident, both models having the same number of adjustable parameters (Table 2).
Figure 4 shows box plots of the distributions of RMSE for water contents and log conductivity for all data sets, comparing the five model settings. The median of logRMSE for the VGM*4 model is about 1.1 and indicates a mismatch between measured and predicted K data which is larger than one order of magnitude. In contrast, the PDI*4 mismatch is about 0.3 on the log scale, reflecting an improvement by a factor of five on the linear scale. The VGM*6 and PDI*4 show almost similar overall performances regarding the logRMSE, although the former is fitted to the data, whereas the latter is a prediction. As a side note, the RMSE is always at least slightly smaller when the conductivity function is predicted in stead of fitted (VGM*4 and PDI*4) as compared to the case where both functions are fitted (VGM*6, PDI*6, and PDI*7). In the former case the two retention parameter α and n are solely adjusted to match the retention data, whereas in the latter case they are adjusted to match both the retention and the conductivity data.

It has long been known that the capillary bundle models are not well suited to predict capillary conductivity for soils with wide pore size distributions (small values for the parameter n in the van Genuchten model).

Figure 3. Comparison of the different model settings as summarized in Table 2. Bars in the bar charts indicate values for RMSE_{logK} for the five applied model settings. 1: VGM*6, 2: VGM*4, 3: PDI*7, 4: PDI*4, 5: PDI*6. RMSE, root mean squared errors; VGM, van Genuchten/Mualem.
This is because very small changes in water content at very small suctions result in large drops in relative conductivity, which must be regarded as model artifact (Durner, 1994). This is clearly seen for the clay loam (soil j) in Figure 3 when \( K_s \) was set to its measured value and the complete conductivity function is predicted (VGM*4 and PDI*4). This shortcoming is still existent in the PDI model, but could be improved by using an explicit air-entry (Ippisch et al., 2006; Vogel et al., 2000), or the clipped integral method proposed by Iden et al. (2015).

4.2. Prediction of Conductivity in the Dry Moisture Range With Available Data in the Moist Range

Very often, for example when the simplified evaporation method (Peters & Durner, 2008b; Schindler, 1980) is used for fine textured soils, information for the non-capillary conductivity is missing. Then the original PDI formulation would not be appropriate. Our new formulation provides reasonable predictions of non-capillary conductivity even if no data in this range exist.

We illustrate this in Figure 5 for the example soils Gilat loam and the PSFC. In the depicted cases, we fitted the models VMG*6 and PDI*6 to all retention data plus capillary conductivity data. The filled circles indicate the data used for fitting and the open circles indicate the data for validating the prediction in the non-capillary range. Contrary to the VGM*6 model, we obtain a good agreement of the PDI*6 predictions with the observed data in the non-capillary range. The PDI*6 scheme is very well suited to evaluate data sets which contain retention data over a wide moisture range, but lack conductivity data in the non-capillary domain. In this case, a complete prediction of the unsaturated conductivity function (including the capillary component) is not required, and the information of the measured conductivity data can be preserved by fitting \( K_s \) and \( r \).

5. Summary and Conclusion

The non-capillary conductivity component of the PDI model, which is based on the Tokunaga (2009) model, is a considerable simplification of the physically-based flow description, as elaborated by Lebeau and Konrad (2010), since it neglects both the molecular component of disjoining pressure isotherm and increasing viscosity near solid surfaces. Our analysis showed that the dependence of the non-capillary conductivity component of the simple PDI model on suction head is nevertheless remarkably similar to that of the comprehensive model of Lebeau and Konrad. The reason for this is that the two neglected processes counter-balance each other. We therefore conclude that the PDI model formulation is well suited to express the hydraulic conductivity function in the non-capillary flow domain. This bears significant potential for variably-saturated flow simulations in dry soil.

Using the physical laws and constants described by Tuller and Or (2005), Tokunaga (2009), and Lebeau and Konrad (2010), the non-capillary conductivity can be predicted on the basis of the water retention charac-

![Box plots showing root mean squared errors for different model settings and data sets.](image)
teristics in the dry moisture range. Following these theories, we propose a prediction of the non-capillary conductivity within the PDI model system. The resulting improved, yet simple, PDI model is applicable effectively on the macroscopic (cm to dm) scale, while its underlying theory is derived from fundamental laws on the pore scale. Our approach reduces the number of adjustable parameters by one compared to the original PDI formulation. The remaining conductivity parameter \( sK \) and \( \tau \) are the same as for the established models, for example, the van Genuchten/Mualem model. The prediction of non-capillary conductivity is particularly important if no conductivity data are available, or if only data in the capillary-dominated range are available. The latter is regularly the case when evaporation experiments are conducted for fine textured soils and suction heads are measured with tensiometers. We emphasize that for predicting the non-capillary conductivity, a realistic knowledge of the water retention characteristics in the dry moisture range is crucial. Therefore, a combination of the simplified evaporation method and the dew point method (Campbell et al., 2007; Kirste et al., 2019) is a good basis to describe both hydraulic functions over the complete moisture range.

**Appendix A**

**A.1. The Lebeau and Konrad Model for Hydraulic Conductivity in Films**

To describe film conductivity, LK use the relation of film thickness (\( \delta \) [m]) and disjoining pressure (\( \Pi \) [m]), called disjoining pressure isotherm (Derjaguin et al., 1987). The disjoining pressure is the difference between the pressure in the gas phase and the liquid film and therefore equals the suction head. Unlike in the original notation, we express \( \Pi \) here as suction head for the sake of brevity. Under some simplifications, the disjoining pressure isotherm can be formulated as the sum of ionic-electrostatic (\( \Pi_\text{e} (\delta) \) [m]) and molecular components (\( \Pi_\text{m} (\delta) \) [m]) (Derjaguin & Churaev, 1974):

\[
\Pi(\delta) = \Pi_\text{e}(\delta) + \Pi_\text{m}(\delta).
\]  

(A1)
For typical soil minerals, the ionic-electrostatic forces are dominant in holding the liquid water in films at a distance $>10$ nm from the mineral surfaces, whereas the molecular forces (van der Waals forces) are dominant in thin films $<10$ nm.

The ionic-electrostatic component of disjoining pressure is given by (Langmuir, 1938):

$$\Pi_e(\delta) = \frac{\pi k_b T}{e Z^2} \frac{\epsilon_0 \epsilon_\infty}{2 \rho g \delta^2}, \quad (A2)$$

where $\epsilon_\infty$ and $\epsilon_0 (C^2 J^{-1} m^{-1})$ are the static relative permittivity of the liquid phase and the permittivity of free space, respectively, $k_b (J K^{-1})$ is the Boltzmann constant, $T$ (K) is the absolute temperature, $e$ (C) is the electron charge, $Z$ is the valence, $\rho$ (kg m$^{-3}$) is the density of liquid water and $g$ (m s$^{-2}$) is the gravitational acceleration constant. If only $\Pi_e(\delta)$ is considered for the disjoining pressure isotherm, the film thickness can be easily described as function of suction head by solving Equation A2 for $\delta$ as done for example by Tokunaga (2009).

The molecular component is given by (Israelachvili, 1992):

$$\Pi_m(\delta) = -\frac{A_H}{6 \pi \eta g \delta^3}, \quad (A3)$$

where $A_H$ (J) is the Hamaker constant, which represents short range interactions (van der Waals interactions) between the solid and the liquid in the range $<10$ nm (Bergström, 1997; Or & Tuller, 2005). Reported values for $A_H$ range from $10^{-30}$ to $10^{-19}$ J (Israelachvili, 1992). LK used an effective value of $6 \times 10^{-20}$ J, which is based on the work of Tuller and Or (2005).

Equations A1–A3 provide a means to calculate the suction head as a function of film thickness. However, there is no simple means to calculate film thickness as a function of suction head, because Equation A1 can’t be solved analytically for $\delta$. Figure A1, adapted from LK, shows the contributions of ionic-electrostatic and molecular components of disjoining pressure in relation to film thickness with the parameters used in LK, given here in Table A1. For $\delta > 10$ nm, the suction head is dominated by the ionic-electrostatic component, which is the basis for the model of Tokunaga (2009). For $\delta < 1$ nm, the molecular component is dominant. In the range between these, both components are significant. This implies that neglecting the molecular component leads to an underestimation of film thickness and thus an underestimate of film conductivity already for suction heads $h > 2$ m ($\delta < 10$ nm).

Based on the relationship between film thickness and suction head, the hydraulic conductivity curve for film-flow can be derived. For thick films, with $\delta > 10$ nm, the average viscosity of the soil solution can be assumed to equal the viscosity of the bulk liquid (Or & Tuller, 2000). Solving the Navier-Stokes equation for these films and using the assumptions of Tokunaga (2009) regarding the perimeter of the solid particles per unit cross-sectional area yields (Lebeau & Konrad, 2010):

$$K_m = \frac{\rho g}{\pi \eta D_e} (1 - \varphi) 4 \delta^3, \quad (A4)$$

where $D_e$ (m) is the equivalent grain diameter (details in Section 2.2.3) and $\varphi$ is the porosity, which are both soil specific parameters. This is essentially the solution of Tokunaga (2009) for $K_m$ as function of film thickness. Tokunaga used only the ionic-electrostatic component of disjoining pressure (Equation A2) and was therefore able to provide a closed-form expression for $K_m$ as function of suction head, yielding the slope of $-1.5$ if $K_m$ is plotted versus the decimal log of suction head. Furthermore, Tokunaga (2009) derived the solution for monodispersed porous media. We note that Tokunaga used a slightly modified expression of Equation A2 from Wan and Tokunaga (1997). LK formulated film conductivity as relative film conductivity, that is, they divided it by $K_e$ to fit in their scheme for total liquid conductivity prediction.

In thin films, the viscosity will increase exponentially with decreasing distance from the solid surface due to short- and long-range interfacial forces (Low, 1979; Or & Tuller, 2000). Neglecting the increasing viscosity near the mineral surfaces leads to an overestimation of film conductivity in thin films. Using this exponential relationship with the constant of Low (1979), Or and Tuller (2000) solved the Navier-Stokes equation for thin films, finally yielding (Lebeau & Konrad, 2010):
for $\delta < 10$ nm, where $B$ is a function of film thickness and temperature given by (Or & Tuller, 2000):

$$B = \left( 4\delta^3 - 5a\delta^2 - a^2\delta \right) \exp\left( -\frac{a}{\delta} \right) - \left( 6a^2\delta + a^3 \right) \text{Ei}\left( -\frac{a}{\delta} \right),$$

where $a = 1.621 \times 10^{-7}/T$ (m). $\text{Ei}(X)$ is the exponential integral $\int_{-\infty}^{X} e^t/tdt$. Since LK (and Modaresi Rad et al., 2020 alike) applied Equation A4 for films $\geq 10$ nm and Equation A5 for films $<10$ nm, there is a discontinuity for $K_{nc}(\delta)$ at $\delta = 10$ nm. This corresponds to a suction head of $\sim 2.5$ m if the parameters in LK are used (Table A1; also used in this study). We note that for large $\delta (>10$ nm), $B$ converges to $4\delta^3$. Therefore, we use Equation A5 with Equation A6 for comparing the PDI non-capillary conductivity function with the LK formulation.

### A.2. Modified Akaike’s Information Criterion

The Akaike information criterion corrected for small sample size, $\text{AIC}_c$ (Akaike, 1974; Hurvich & Tsai, 1989) is defined as:
Modified Akaike’s Information Criterion for All Combinations of Model Settings and Data Sets

|        | VGM*6 | VGM*4 | PDI*7 | PDI*4 | PDI*6 |
|--------|-------|-------|-------|-------|-------|
| Silt loam | 8.06  | 9.97  | −17.28 | −4.00 | −18.14 |
| Clay loam  | 35.19 | 88.18 | −2.03  | 57.73 | 1.39   |
| Minasny loam | −188.43 | 234.94 | −247.97 | −86.32 | −130.31 |
| Sandy loam | 42.71 | 75.43 | 20.44  | 44.03 | 21.55  |
| GILAT | 90.28 | 114.08 | −37.66 | −16.75 | −24.30 |
| PFSC | 54.25 | 98.20 | −30.59 | 12.51 | −20.16 |
| Berlin sand | −109.17 | 197.01 | −140.12 | −121.70 | −133.30 |
| REHOVOT | 43.16 | 38.31 | 25.39  | 33.63 | 27.10  |
| Minasny sand | −83.93 | 298.27 | −196.54 | −120.85 | −90.28 |
| Schindler sand | −121.83 | 223.79 | −276.24 | 87.75 | −171.81 |

\[
AIC_c = -2\mathcal{L} + 2k + \frac{2k(k + 1)}{n - k - 1}
\]

where \( \mathcal{L} \) is the log-likelihood, \( n \) is the number of data, and \( k \) is the number of estimated model parameters. For calculating the log-likelihood, we assumed independently normally distributed error with a standard deviation of 0.01 for the water content and 0.25 for the common log of hydraulic conductivity in \((\text{cm} \text{ d}^{-1})\).

The values of the AIC\(_c\) for all models and datasets are given in Table A2.

## Data Availability Statement

The 10 data sets used in this study are collected from the published literature and are available as follows. Sandy Loam & Clay Loam (originally published in Pachepsky et al., 1984); Tuller and Or (2001); Silt Loam (originally published in Pachepsky et al., 1984); Zhang (2011); PFSC, Rehovot Sand & Gilat Loam: Mualem (1976b); Minasny Sand & Minasny Loam: Minasny and Field (2005); Schindler Sand: Schindler and Müller (2006); Berlin Sand: Peters (2013).

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