Improved Prediction of Hydraulic Conductivity With a Soil Water Retention Curve That Accounts for Both Capillary and Adsorption Forces

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Abstract  Hydraulic conductivity curves (HCCs) are important inputs in land surface modeling. The general way for predicting an HCC from a soil water retention curve (SWRC) requires an additional input of the saturated hydraulic conductivity. However, the macro effect near saturation often results in difficulty and poor performance when predicting the conductivity. In this paper, we introduce a novel method for predicting the HCC fully from the SWRC, requiring no additional parameters. This is achieved by applying an estimated conductivity (from the SWRC) in the dry range as a new matching point, in addition to modifying an existing HCC model that accounts for both capillary and adsorption forces. Testing with a total of 159 soil samples indicated that the new model substantially improves the prediction of the HCC in compared with the model with the input of the saturated hydraulic conductivity, with the $R^2$ increased from 0.48 to 0.76 and the root-mean-square error value reduced from 1.60 to 0.81 cm d$^{-1}$. The abrupt drop near saturation of the HCC model for soils with small $n$ values close to 1.0, which is a parameter used in shaping the SWRC, was also overcome by forcing the water content be saturated above a fixed potential of −1 cm.

1. Introduction

Hydraulic conductivity properties are frequently required in water and solute transport simulation. However, the measurement of the hydraulic conductivity curve (HCC) is generally difficult and time-consuming. In practice, the HCC is physically or empirically related to, and then can be predicted from the soil water retention curve (SWRC) through the integration of flux in the interconnected capillary tubes (e.g., Alexander & Skaggs, 1986; Burdine, 1953; Mualem, 1976). Among the different methods, the most popular one might be the framework provided by Mualem (1976). Specifically, this built relationship is for the relative hydraulic conductivity. To describe the actual HCC, a matching point, which is usually taken at the saturated hydraulic conductivity $K_s$, is required.

The use of $K_s$ as the matching point, in spite of the wide acceptance, can cause significant deviation from the unsaturated conductivity observations. Schaap and Leij (2000) and Schaap et al. (2001) demonstrated that applying the observed $K_s$ as the matching point leads to overestimation of the conductivity at most matric potentials. The reason for this, as discussed in detail by van Genuchten and Nielsen (1985), is that $K_s$ is sensitive to macropore flow, while unsaturated flow occurs in the soil matrix. Van Genuchten and Nielsen (1985) therefore argued that the matching point should ideally be located at a point below saturation.

The advances in soil hydraulic property modeling suggest that, by including the impact of adsorption forces, the developed models can describe the soil hydraulic properties well, from saturation to oven-dryness (e.g., Lebeau & Konrad, 2010; Tuller & Or, 2001; Wang et al., 2013, 2016). In the dry range, where adsorption forces dominate, the unsaturated hydraulic conductivity is controlled by the film thickness and the specific surface area (Bird et al., 1960; Tokunaga, 2009). As the film thickness can be estimated from the matric potential (Tokunaga, 2009, 2011), and the specific surface area estimated from the SWRC (Tuller & Or, 2005), the hydraulic conductivity that accounts for adsorption forces can thus be directly estimated from the known SWRC. This method, which was first proposed by Lebeau and Konrad (2010), has performed very well in hydraulic conductivity estimation in a series of applications (Wang et al., 2017, 2018, 2019). Therefore, since the prediction of an HCC requires only one matching point, the question is whether this estimated conductivity under dry conditions can be applied as a better matching point than $K_s$ in hydraulic conductivity prediction.
To apply the estimated conductivity under dry conditions as the matching point, the hydraulic conductivity function must capture the impact of capillary and adsorption forces in a single continuous expression. The combination models, as presented in, for example, Lebeau and Konrad (2010), Zhang (2011), Wang et al. (2016), Liao et al. (2018), and Stanić et al. (2020), among others, used different formulas to describe the capillary- and adsorption-associated conductivities. The conductivities in the wet range showed no tight connection with those in the dry range. Therefore, for these combined models, the estimated conductivity under dry conditions cannot be applied as the matching point.

Differing from these combination models, Wang et al. (2018) presented a continuous formula to describe the HCC and applied the Fredlund and Xing (1994) model to describe the SWRC over the entire moisture range. The model is hereafter referred to as the FXW model. The HCC of the FXW model showed a similar form to the commonly used van Genuchten (1980)-Mualem (1976) model (hereafter referred to as the VGM model), and required no additional parameters in predicting the HCC. The HCC is written as:

$$K = K_s \left( \frac{\Gamma - \Gamma (h_0)}{1 - \Gamma (h_0)} \right)^l \left[ 1 - \left( 1 - \Gamma^{1/m} \right)^{1-1/n} \right]^2$$  (1)

where $h_0$ is the matric potential corresponding to zero water content, which is set as $-6.3 \times 10^6$ cm, according to Schneider and Goss (2012); $l$ is an empirical factor, which has a typical value of 3.5, as suggested by Wang et al. (2018); and $\Gamma(h)$, $m$, and $n$ are represented in the SWRC provided by Fredlund and Xing (1994), which is written as:

$$S(h) = \left[ 1 - \frac{\ln(1 + h/h_r)}{\ln(1 + h_0/h_r)} \right] \Gamma(h)$$  (2)

and $\Gamma(h)$ is written as:

$$\Gamma(h) = \left( \ln \left( e + |ah|^{n} \right) \right)^{-m}$$  (3)

where $S = \theta/\theta_s$ is the saturation degree, with $\theta$ ($L^3$ $L^{-3}$) being the volumetric water content and $\theta_s$ ($L^3$ $L^{-3}$) being the saturated water content; $h$ ($L$) is the matric potential; $a$ ($L^{-1}$) is the fitted parameter, and $h_r$ was interpreted originally as the matric potential corresponding to the residual water content by Fredlund and Xing (1994). When not applying the definition of the so-called residual water content (Wang et al., 2018), $h_r$ is simply regarded as a shape parameter, and is set to $-1.5 \times 10^3$ cm, following Fredlund and Xing (1994). It should be noted that $h_r$ is incorrectly written as $-1.5 \times 10^2$ cm in the text in Wang et al. (2018), although the performance of Equation 2 is not sensitive to the value of $h_r$ (Wang et al., 2017).

Equation 1 shows that, with the estimated hydraulic conductivity in the dry range, $K_s$ and then the HCC can be predicted because all the other parameters that are required are determined from the known SWRC (Equation 2).

The original HCC of the FXW model does have one limitation. That is, the HCC described in Equation 1 drops abruptly near saturation and yields poor agreement with the observations when parameter $n$ approaches the lower limit of 1 (de Rooij et al., 2021; Wang et al., 2018). This shortcoming, which is frequently seen in soil hydraulic models, results from the non-zero $d \theta/dh$ at the matric potential of zero (de Rooij et al., 2021; Schaap & Van Genuchten, 2006; van Genuchten & Nielsen, 1985). The non-zero slope at saturation (i.e., the zero air-entry value) implies the existence of infinite pores, which is unrealistic. For the VGM model, a simple solution, as provided by Vogel et al. (2000) and Ippisch et al. (2006), is to force the water content to be saturated above a small and fixed water potential value.

The aim of this study was to: (a) apply the simple method provided by Vogel et al. (2000) and Ippisch et al. (2006) to improve the prediction of hydraulic conductivity, with the FXW model used for soils with small $n$ values; and (b) to test whether the estimated conductivity in the dry range can be used as a matching point for HCC prediction.

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2. Theory Development

2.1. Improved Description of Soil Hydraulic Conductivity Near Saturation—The FXW-M1 Model

Following Vogel et al. (2000) and Ippisch et al. (2006), a fixed potential of \( h_s \) is introduced to improve the performance of the FXW model near saturation. This modified model is hereafter referred to as the FXW-M1 model. The modified SWRC of the FXW-M1 model is written as:

\[
\theta = \begin{cases} 
\theta_s & \text{for } h < h_s \\
\frac{1 - \ln(1 + (h - h_s)/h_r)}{\ln(1 + (h_0 - h_s)/h_r)} \Gamma(h) / \Gamma(h_s) & \text{for } h \geq h_s 
\end{cases}
\]  

(4)

with \( \Gamma(h) \) being:

\[
\Gamma(h) = (\ln(e + |\alpha_h h_s^n|))^{-\alpha}
\]  

(5)

The modified HCC of the FXW-M1 model is expressed as:

\[
K = \begin{cases} 
K_s \left( \frac{\Gamma(h) - \Gamma(h_0)}{\Gamma(h_s) - \Gamma(h_0)} \right)^2 \left[ 1 - \left( 1 - \frac{\Gamma(h)}{\Gamma(h_s)} \right)^{1-1/\alpha} \right]^{-2} & \text{for } h < h_s \\
K_s & \text{for } h \geq h_s
\end{cases}
\]  

(6)

The SWRC and the HCC, as described in Equations 4 and 6, reduce to the original FXW model when \( h_s \) has the value of 0.

The illustration in Figures 1b and 1d shows that, when the value of \( n \) approaches the lower limit of 1, the HCC of the original FXW model drops dramatically just below saturation. For example, a small decrease in the saturation degree just below saturation for \( n \) being 1.1 results in a considerably decrease of the relative hydraulic conductivity from 1 to about 0.2. This unrealistic decrease coming from the model structure results in underestimation of the conductivity. To overcome this shortcoming, Wang et al. (2018) suggested using a lower boundary of 1.2 for parameter \( n \), which, however, results in a loss of accuracy in describing the SWRC.

By introducing a non-zero water potential of \( h_s \), the HCC of the FXW-M1 model presents a much smoother decrease. For small values of \( n \) close to 1, the difference between the FXW-M1 model and the original FXW model is significant. Meanwhile, for large values of \( n \) close to about 2, the difference between these two models becomes negligible (Figure 1b).

Figure 1d indicates that the improved description of the HCC near saturation can be achieved with an \( h_s \) value that is only slightly less than 0. The more negative \( h_s \) is, the smoother the drop of the HCC near saturation. When it comes to the SWRC, a more negative \( h_s \), however, yields a non-decreasing water content over a longer matric potential range. For example, by setting \( h_s \) to \(-2 \) cm, following Vogel et al. (2000), the modified SWRC described in Equation 4 deviates significantly from the original FXW model near saturation (Figure 1c). The optimal value for \( h_s \) will be determined in Section 4.1.

2.2. Prediction of the HCC Fully From the SWRC—The FXW-M2 Model and the FXW-M2-l Model

In this section, we demonstrate the method for predicting the HCC fully from the SWRC, through the introduction of a new matching point that can estimated directly from the SWRC. When applying the default value of 3.5 for parameter \( l \), the developed model is hereafter referred to as the FXW-M2 model. When applying the optimized value of \( l \) derived for each soil type, the model is hereafter referred to as the FXW-M2-l model.

The hydraulic conductivity that accounts for adsorption forces is determined by the specific surface area \( S_A \) (\( L^2 \) \( L^{-3} \)) and the film thickness \( f \) (Bird et al., 1960). It can be expressed as (Lebeau & Konrad, 2010; Wang et al., 2017):

\[
K_f(\theta) = B(f) \frac{2\rho g S_A}{3\pi \eta} f^3
\]  

(7)
where \( \rho \) is the water density (9.98 \times 10^2 \text{ kg m}^{-3} ), \( g \) is the acceleration of gravity (9.81 \text{ m s}^{-2} ), and \( \eta \) is the fluid viscosity (1.005 \times 10^{-3} \text{ Pa s at 293 K} ). \( B(f) \) is introduced as a correction factor that accounts for the modified viscosity for a film thickness of less than 10 nm (Lebeau & Konrad, 2010; Or & Tuller, 2000). \( B(f) \) is expressed as:

\[
B(f) = \left( (4f^3 - 5af^2 - a^3 f) \exp \left( -\frac{a}{f} \right) - (6a^2 f + a^3) \text{Ei} \left( -\frac{a}{f} \right) \right) / (4f^3)
\]  

(8)

where \( a \) is 5.53 \times 10^{-10} \text{ m at 293 K}, and \( \text{Ei}(-x) = -\int_{x}^{\infty} \text{exp}(-t)/t \text{d}t \) is the exponential integral. The film thickness \( f \) is controlled by both the electrostatic forces and the van der Waals forces. The relationship between the matric potential \( h \) and film thickness \( f \) is expressed as:

\[
h(f) = h_s(f) + h_{\text{os}}(f)
\]  

(9)

where \( h_s(f) \) is the matric potential that accounts for the impact of the electrostatic forces, as written in Langmuir (1938) and Tokunaga (2009):
\[
\theta_s = \frac{h_s}{h_m} = \theta_t \left[ 1 - \ln \frac{h_s/h_t}{h_m/h_t} \right] \frac{\Gamma (h_m) / \left( \frac{A_{svl}}{6\pi \rho g h_m} \right)^{1/3}}{\Gamma (h_t)} 
\]

where \( \theta_s \) is the soil water content; \( h_s \) is the film thickness, \( h_m \) is the matric potential; and \( h_t \) is the saturated hydraulic conductivity. The calculation of the film thickness can be approximately divided into the three terms: \( A_{svl} \), \( 6\pi \rho g f^3 \), and \( \frac{1}{\rho g f^3} \). The first term \( A_{svl} \) can be directly estimated by Equation (11). The second term \( 6\pi \rho g f^3 \) represents the film thickness, which can be directly estimated by Equation (10). The third term \( \frac{1}{\rho g f^3} \) represents the relative permittivity of free space, which is set to 8.85 × 10^{-12} C^2 J^{-1} m^{-1}.

\[
h_s(f) = -\left( \frac{\epsilon_0 \epsilon_r}{2} \right) \left( \frac{\pi k_B T}{2e_c} \right) \frac{1}{\rho g f^2} 
\]

where \( \epsilon \) is the relative permittivity of water (78.54); \( \epsilon_r \) is the permittivity of free space (8.85 × 10^{-12} C^2 J^{-1} m^{-1}); \( k_B \) is the Boltzmann constant (1.381 × 10^{-23} J K^{-1}); \( T \) is the Kelvin temperature; \( e \) is the ion valence, which was set to 1 following Tokunaga (2009) and Lebeau and Konrad (2010); and \( e_c \) is the electron charge (1.602 × 10^{-19} C).

\( h_s(f) \) is the matric potential that represents the impact from the van der Waals forces, which is expressed as (Iwamatsu & Horii, 1996):

\[
h_{svl}(f) = \frac{A_{svl}}{6\pi \rho g f^3} 
\]

where \( A_{svl} \) is the Hamaker constant for solid-vapor interactions, which is set to \(-6.0 \times 10^{-20}\) J, following Tuller and Or (2005). It should be noted that to derive the film thickness \( f \), Equation (9) has to be solved numerically.

The \( S_A \) in Equation 7 can be approximately estimated by dividing the soil water content by the film thickness, as suggested by Tuller and Or (2005), assuming that the soil water content is totally in film form under very dry conditions. Here, taking a typical matric potential \( h_m \) where the van der Waals forces dominate, the specific surface area can be estimated approximately as (Tuller & Or, 2005):

\[
S_A = \frac{\theta_m}{f_m} = \theta_t \left[ 1 - \ln \frac{h_s/h_m}{h_s/h_t} \right] \frac{\Gamma (h_m) / \left( \frac{A_{svl}}{6\pi \rho g h_m} \right)^{1/3}}{\Gamma (h_t)} 
\]

For the introduce of \( h_s \) has negligible impact on the estimation of \( \theta_m \) in very conditions, for simplicity, \( h_s \) is neglected in deriving \( S_A \). It should be noted that Equation 12 does not account for the impact of the electrostatic forces directly. That is, the film thickness \( f_m \) is derived directly from Equation 11. The reason, as discussed in Tokunaga (2011), is that the impact of the electrostatic forces might be empirically represented in the parameter \( A_{svl} \).

With the film thickness estimated numerically from Equation 6 and with substitution of all the other parameters, the calculated hydraulic conductivity by Equation 7 is reduced to:

\[
K(h) = B(f) \frac{2\rho g}{3\pi} f^3 \theta_t \left[ 1 - \ln \frac{h_s/h_m}{h_s/h_t} \right] \frac{\Gamma (h_m) / \left( \frac{A_{svl}}{6\pi \rho g h_m} \right)^{1/3}}{\Gamma (h_t)} 
\]

where \( b(h) \) represents the combined impact of the film thickness, the specific surface area and the correction factor that accounts for the modified viscosity. When taking the matric potential at \( h_m = -1.0 \times 10^5 \) cm, \( b(h_m) \) has a value of 2.693 × 10^{-6} cm d^{-1}. When the SWRC is known, the corresponding hydraulic conductivity \( K(h_m) \) can be directly estimated by Equation 13.

\[
K(h_m) = \theta_t b(h_m) \Gamma (h_m) \left( \frac{\Gamma (h_m) - \Gamma (h_0)}{\Gamma (h_m) - \Gamma (h_0)} \right)^{1/3} \left[ 1 - \left( \frac{1 - \Gamma (h_0)^{1/\alpha}}{1 - \Gamma (h_0)^{1/\alpha}} \right)^{1/\alpha} \right] ^2 
\]

Substituting the estimated \( K(h_m) \) back into Equation 6 gives the HCC of the FXW-M2 model, written as: To avoid the confusion with the observed one, written as.
\[ K = \begin{cases} 
\frac{\theta_s(h_m) \Gamma(h_m)}{\Gamma(h_s) - \Gamma(h_0)} \left( \frac{\Gamma(h) - \Gamma(h_0)}{\Gamma(h_m) - \Gamma(h_0)} \right)^l \left[ 1 - \left(1 - \Gamma(h)^{1/n}\right)^{1-1/n} \right]^{2} & h < h_s \\
\frac{\theta_s(h_m) \Gamma(h_m)}{\Gamma(h_s) - \Gamma(h_0)} \left( \frac{\Gamma(h) - \Gamma(h_0)}{\Gamma(h_m) - \Gamma(h_0)} \right)^l \left[ 1 - \left(1 - \Gamma(h)^{1/n}\right)^{1-1/n} \right]^{2} & h \geq h_s 
\end{cases} \]  

Compared to Equation 6, the new HCC described in Equation 15 requires no additional parameters, other than those applied in describing the SWRC (\(l\) has a constant value of 3.5). That is, the new HCC can be fully predicted from the SWRC.

An illustration of the FXW-M2 model shows that the predicted conductivity in the dry range is mainly controlled by the corresponding water content, that is, the higher the water content, the higher the conductivity (Figure 2b). In the wet range, in contrast, the predicted conductivity is generally much higher for coarse-textured soils.
Table 1
The Upper and Lower Boundaries of the Optimized Parameters in Deriving
the Optimal $h_s$

| Parameter | The lower boundary | The upper boundary |
|-----------|--------------------|--------------------|
| $a$ (cm$^{-1}$) | 0.001 | 0.1 |
| $n$ | 1.01 | 10.00 |
| $m$ | 0.01 | 1.5 |
| $\theta_s$ | 0.24 | 0.65 |
| $K_s$ (cm d$^{-1}$) | $1.0 \times 10^{-4}$ | $1.0 \times 10^4$ |

3. Materials and Methods

3.1. Data Sets

Data sets from the UNsaturated SOil hydraulic DAtabase (UNSODA) (Nemes et al., 2001) were applied to evaluate the model performance. Since the determination of $K(h_s)$ relies on the accurate estimation of $\theta_m$ in dry range, the applied SWRC should cover measurements in a very dry range. In this study, we only selected the data with the measured matric potential reaches a lower boundary of $-1.0 \times 10^4$ cm set for, resulting in a total of 159 soil samples.

3.2. Parameter Optimization to Define $h_s$

For we intend to predict HCC from SWRC, it is better to fix $h_s$ at a value for all soil samples. The optimal value for $h_s$ was derived by minimizing the mean root-mean-square error of the SWRC and the HCC. Following Schiap and Van Genuchten (2006), $h_s$ was assumed to be in a range from $-20$ to $0$ cm, and for each selected $h_s$, the SWRC and the HCC were fitted with observations.

For the SWRC, as described in Equation 4, the objective function $\Phi(p)$ to be minimized is defined as:

$$\Phi(p) = \sum_{i=1}^{n_p} \left[ \theta_i - \bar{\theta}_i(p) \right]^2$$

(16)

where $n_p$ is the number of data pairs for the retention; and $\theta_i$ and $\bar{\theta}_i$ are the measured and the fitted water content, respectively, $p = (a, n, m, \theta_s)$ is the parameter vector used for the optimization. It should be noted that $\theta_s$ is only optimized when there is no observation, and the optimal value is set to be no less than the highest water content observation.

For the HCC (Equation 6) optimization, the objective function is:

$$\Phi_K(p_K) = \sum_{i=1}^{n_p} \left[ \log_{10}(K_i) - \log_{10} \left( \bar{K}_i(p_K) \right) \right]^2$$

(17)

where $K_i$ and $\bar{K}_i$ are the measured and the fitted conductivity, respectively, $p_K = (K_s, l)$ is the parameter vector used for the optimization. The reason for treating $K_s$ as a free fitted parameter is that the observed value is impacted by the presence of macroporosity. It should be noted that the HCC is only fitted when deriving the optimal $h_s$.

The optimization was done by applying the shuffled complex evolution (SCE-UA) method developed at the University of Arizona, as proposed by Duan et al. (1992). The SCE-UA method is a general-purpose global optimization program, which is widely applied in hydrological model calibration (e.g., Gupta et al., 2009; Wang et al., 2018, among many others). In searching for the global optimum, it applies a systematic competitive evolutionary process in evolving clusters of samples drawn from the parameter space. The optimization process is stopped either when the normalized geometric range of the parameters is less than 0.001 or the change of the objective function is less than 10% in the last 10 shuffling loops. Table 1 defines the upper and lower boundaries of the optimized parameters.
To evaluate the model performance, the root-mean-square error (RMSE) and the coefficient of determination \( R^2 \) are introduced. The RMSE is defined as:

\[
RMSE = \sqrt{\frac{1}{N} \sum_{i=1}^{N} (o_i - \bar{o}_i)^2}
\]  

(18)

where \( N \) represents the number of data pairs; and \( o_i \) and \( \bar{o}_i \) are the measured and estimated values, respectively. In terms of conductivity, the log-scale value is applied. \( R^2 \) is defined as:

\[
R^2 = 1 - \frac{\sum_{i=1}^{N} (o_i - \bar{o}_i)^2}{\sum_{i=1}^{N} (o_i - \bar{o})^2}
\]  

(19)

where \( \bar{o} \) is the mean value of \( o_i \).

The optimal value for \( h_s \) is therefore selected as the one yielding the lowest mean RMSE for both the SWRC and HCC.

3.3. Prediction of the HCC

With the optimal \( h_s \) determined, the SWRC is fitted with the observations to derive the parameters \( \alpha, n, m, \) and \( \theta_s \). The HCC can then be predicted. In prediction of the HCC, four models were applied, including the FXW, the FXW-M1, the FXW-M2 and the FXW-M2-l models. The observed \( K_s \) is applied as the matching point for the FXW and the FXW-M1 models, while the estimated \( K(h_m) \) is used for the FXW-M2 and the FXW-M2-l models. It should be noted that \( l \) is only optimized for the FXW-M2-l model while it is set to 3.5, as suggested by Wang et al. (2018), for the other three models. Table 2 shows all the optimized and fitted parameters for the four models.

4. Results

4.1. Optimized Value for \( h_s \)

Figure 3a shows that the mean RMSE for the SWRC is nearly constant for \( h_s \) varying from 0 to about \(-1.0 \) cm, after which the value increases rapidly for all soil types, but especially for the sand and loam soils. The reason is that the coarse-textured soils have a much higher air-entry value.

For the HCC, a small decrease of \( h_s \) yields a sharp decrease of the mean RMSE value. For \( h_s \) of less than \(-1.0 \) cm, the decrease of RMSE becomes very smooth. The optimal value differs slightly for the different soil types. For example, a value of \(-3.0 \) cm for \( h_s \) shows the lowest RMSE for sand soils, while the value of \(-10.0 \) cm performs the best for loam soils.

Since a value of \( h_s \) of less than \(-1.0 \) cm only improves the performance for the HCC slightly, while yielding a much poorer performance for the SWRC, we suggest an optimal value of \(-1.0 \) cm for \( h_s \). This optimal value is much higher than the value of \(-4.0 \) cm for the modified VGM model, as suggested by Schaap and Van Genuchten (2006). The different values can be attributed to the different model structures of the FXW-M1 model and the modified VGM model.
4.2. Prediction of the Hydraulic Conductivity

In this section, we describe the predictions of hydraulic conductivity obtained with different matching points. Both the FXW model and the FXW-M1 model apply the observed $K_s$ as the matching point. For the FXW-M2 model and the FXW-M2-l model, the matching point is derived from the fitted SWRC, as illustrated in Section 2.2.

Figure 4 presents the predictions obtained for all the soil samples, while in Figures 5–10, the predictions for each soil type are shown. For each soil type, we also provide the prediction obtained with the optimal $l$ value, as represented by the FXW-M2-l model.

For all the evaluated soil samples, the original FXW model provided in Wang et al. (2018) performs relatively poorly in predicting the HCC (Figure 4a), with the $R^2$ and $\text{RMSE}_{\log 10(K)}$ being 0.48 and 1.60 cm d$^{-1}$, respectively. For most samples, this model tends to overestimate the conductivity for an observed conductivity.
higher than about 0.01 cm d\(^{-1}\), whereas it underestimates the conductivity for smaller observed conductivity values. The corresponding water potential is about −100 cm for this critical conductivity (Figures 5b, 5d, 5f, and 5h). As shown in Figure 5b, the FXW model significantly underestimates the conductivity for soils with an \( n \) value close to 1.0.

Compared to the FXW model, the FXW-M1 model, with the introduction of the fixed \( h_s \), improves the overall prediction. The reported \( R^2 \) increases from 0.75 (the FXW model) to 0.81, and the \( \text{RMSE}_{\log(K)} \) decreases from 1.20 (the FXW model) to 0.89 cm d\(^{-1}\). However, as with the FXW model, the FXW-M1 model overestimates the conductivity in the wet range while underestimating the conductivity in the dry range, for most samples (Figure 5c). The figures for the individual soil samples, as presented in the right panel, show that, for \( n \) values higher than about 1.25, the FXW-M1 model performs almost the same as the FXW model.

When applying the estimated \( K(h_m) \) as a new matching point, the FXW-M2 model further improves the prediction, with the reported \( R^2 \) being 0.85 and the \( \text{RMSE}_{\log(K)} \) being 0.80 cm d\(^{-1}\). Specifically, the FXW-M2 model improves the prediction mainly for observed conductivity values of higher than about 0.01 cm d\(^{-1}\) (Figure 5e). In the dry range, the FXW-M2 model underestimates the conductivity (Figures 5e, 5f, and 5h). Figure 5g presents the prediction obtained with the optimal \( l \) value. Here, for the selected sand soils, the optimal value of \( l \) is the same as the default value of 3.5, as suggested by Wang et al. (2018).

### 4.2.2. Sandy Loam Soils

As with the sand soils, the FXW model shows the worst performance for the sandy loam soils, with the overall \( R^2 \) being 0.53 and the \( \text{RMSE}_{\log(K)} \) being 1.60 cm d\(^{-1}\). For many soils with \( n \) values close to 1.0, the FXW model significantly underestimates the conductivity (Figures 6a and 6b). The FXW-M1 model increases the \( R^2 \) greatly from 0.53 (the FXW model) to 0.74. However, it tends to overestimate the conductivity for almost all the samples (Figures 6b, 6c, 6d, 6f, and 6h), indicating the presence of macropores near saturation.

Compared to the FXW-M1 model, the FXW-M2 model reduces the \( \text{RMSE}_{\log(K)} \) from 1.20 to 0.87 cm d\(^{-1}\), indicating that the estimated \( K(h_m) \) is a much better matching point than the observed \( K_s \) for sandy loam soils. However, the FXW-M2 model tends to slightly underestimate the conductivity (Figure 6e). With an optimal \( l \) value of 4.00, the FXW-M2 model further improves the prediction (Figures 6b, 6g, and 6h).

**Figure 4.** Prediction of the conductivity with the different models for all the soil samples. The data density is represented by different color. The higher the value, the more samples are included.
Figure 5. Predictions of the hydraulic conductivity with the different models for sand soils. The optimal $l$ value for sand soils is also 3.50 for the FXW-M2-I model (g). In the first column, all soil samples included in the selected soil type are used while in the second column, we selected four individual soil samples in the soil type to demonstrate the predicted HCCs with four different models. The data density in the first column is represented by different color. The higher the value, the more samples are included.
Figure 6. Predictions of the hydraulic conductivity with the different models for sandy loam soils. The optimal \( l \) value for sandy loam soils is 4.00 for the FXW-M2-I model (g). In the first column, all soil samples included in the selected soil type are used while in the second column, we selected four individual soil samples in the soil type to demonstrate the predicted HCCs with four different models. The data density in the first column is represented by different color. The higher the value, the more samples are included.
Figure 7. Predictions of the hydraulic conductivity with the different models for loam soils. The optimal $l$ value for loam soils is 4.38 for the FXW-M2-I model (g). In the first column, all soil samples included in the selected soil type are used while in the second column, we selected four individual soil samples in the soil type to demonstrate the predicted Hydraulic conductivity curves (HCCs) with four different models. The data density in the first column is represented by different color. The higher the value, the more samples are included.
Figure 8. Predictions of the hydraulic conductivity with the different models for silty loam soils. The optimal $l$ value for silty loam soils is 3.96 for the FXW-M2-I model (g). In the first column, all soil samples included in the selected soil type are used while in the second column, we selected four individual soil samples in the soil type to demonstrate the predicted Hydraulic conductivity curves (HCCs) with four different models. The data density in the first column is represented by different color. The higher the value, the more samples are included.
Figure 9. Predictions of the hydraulic conductivity with the different models for silty clay soils. The optimal $l$ value for silty clay soils is 2.80 for the FXW-M2-I model (g). In the first column, all soil samples included in the selected soil type are used while in the second column, we selected four individual soil samples in the soil type to demonstrate the predicted Hydraulic conductivity curves (HCCs) with four different models. The data density in the first column is represented by different color. The higher the value, the more samples are included.
Figure 10. Predictions of the hydraulic conductivity with the different models for clay soils. The optimal $l$ value for clay soils is 4.13 for the FXW-M2-I model (g).

In the first column, all soil samples included in the selected soil type are used while in the second column, we selected four individual soil samples in the soil type to demonstrate the predicted Hydraulic conductivity curves (HCCs) with four different models. The data density in the first column is represented by different color. The higher the value, the more samples are included.
4.2.3. Loam Soils

Figure 7 shows that the predictions of conductivity with the different models for loam soils are very similar to those for sandy loam soils. The FXW model shows significant underestimation of the conductivity, while the FXW-M1 model, although it improves the prediction greatly, tends to overestimate the conductivity (Figures 7a and 7c). When the FXW-M2 model shows a superior performance, with the \( R^2 \) being 0.84 and the \( \text{RMSE}_{\log(K)} \) being 0.91 cm d\(^{-1}\), it slightly underestimates the conductivity for almost all the samples (Figures 7b, 7d, 7e, 7f, and 7h). In contrast, an optimal \( l \) value of 4.38 reduces the \( \text{RMSE}_{\log(K)} \) greatly, from 0.91 (with the default \( l \) value of 3.50) to 0.59 cm d\(^{-1}\).

4.2.4. Silty Loam Soils

In general, the model performance for silty loam soils is similar to that for sandy loam and loam soils. Overall underestimation is found for the FXW model, while overall overestimation is apparent for the FXW-M1 model (Figures 8a and 8c). However, for silty loam soils, the FXW-M1 model yields a higher \( \text{RMSE}_{\log(K)} \) of 1.50 cm d\(^{-1}\), compared to the 1.40 cm d\(^{-1}\) of the FXW model, although it increases the \( R^2 \) from 0.55 (the FXW model) to 0.60.

Compared to the FXW-M1 model, the FXW-M2 model improves the prediction significantly. The \( R^2 \) is increased from 0.60 (the FXW-M1 model) to 0.86 (the FXW-M2 model), while the \( \text{RMSE}_{\log(K)} \) is reduced from 1.50 to 0.61 cm d\(^{-1}\). However, Figure 8e clearly shows that the FXW-M2 model underestimates the conductivity when the observed conductivity is higher than about 1.0 cm d\(^{-1}\). The corresponding matric potential is in the magnitude of negative tens of centimeters (Figures 8b, 8d, 8f, and 8h). As shown in Figure 8g, when treating \( l \) as a fitting parameter, the FXW-M2-I model still yields underestimation in the high water saturation range.

4.2.5. Silty Clay Soils

All four models perform relatively poorly for silty clay soils, as shown in Figure 9. Figure 9a shows that the FXW model with the matching point of \( k_r \) fails to predict the conductivity for silty clay soils, with the \( R^2 \) being as low as 0.049. The FXW-M1 model presents overall overestimation of the conductivity, with the highest \( \text{RMSE}_{\log(K)} \) of 2.10 cm d\(^{-1}\) (Figure 9c). Although the FXW-M2 model reduces the \( \text{RMSE}_{\log(K)} \) from 2.10 (the FXW-M1 model) to 1.10 cm d\(^{-1}\), it underestimates the conductivity for observed conductivity higher than about 0.01 cm d\(^{-1}\), while overestimating the conductivity for smaller observations (Figure 9e). Because a higher \( l \) would yield an overall higher prediction of conductivity, the FXW-M2-I model only slightly improves the prediction when applying an optimal \( l \) value (Figure 9g).

4.2.6. Clay Soils

Compared to the overall underestimation of the FXW model and the overestimation of the FXW-M1 model, the FXW-M2 model improves the prediction greatly for clay soils. The reported \( R^2 \) is 0.82 and the \( \text{RMSE}_{\log(K)} \) is 0.90 cm d\(^{-1}\). However, with the default value of 3.50 for \( l \), the FXW-M2 model slightly underestimates the conductivity for clay soils (Figures 10d, 10e, and 10f). When applying the optimal value of 4.13, the FXW-M2 further reduces the \( \text{RMSE}_{\log(K)} \) to 0.79 cm d\(^{-1}\) (Figures 10d, 10f, and 10g). This is different from silty loam and silty clay soils, where obvious underestimation of conductivity is found near saturation (Figures 8 and 9).

5. Discussion

5.1. The Impact of the Model Structure

As shown in Section 4.2, the original FXW model provided in Wang et al. (2018) performs relatively poorly in predicting the HCC, and it notably underestimates the conductivity for most samples. This differs from the findings of Schaap and Leij (2000) and Schaap et al. (2001), where applying \( k_r \) as the matching point for the VGM model generally led to overestimated hydraulic conductivity at most matric potentials. This difference is because nearly half of the evaluated soils in this study have a small \( n \) value close to 1 when fitting the SWRC. For this small \( n \) value, the prediction with the original HCC (Equation 1) drops dramatically just below saturation, as shown in Figures 1b and 1d, thus underestimating the conductivity.

By introducing a fixed water potential of \( h_w \), the modified FXW-M1 model improves the performance when compared with the original FXW model, especially for sand soils, sandy loam soils, and loam soils. Nevertheless,
the modified FXW-M1 model with the matching point of $K_m$ overestimates the conductivity for most samples, which is consistent with the findings in Schaap and Leij (2000) and Schaap et al. (2001). This overestimation can be explained by the presence of macropores near saturation, while the matrix flow is controlled by micropores (Schaap & Van Genuchten, 2006).

5.2. The Impact of Macroporosity

When applying the new matching point of $K(h_m)$ instead of $K_m$, the FXW-M2 model improves the prediction considerably for all soil types, with much lower $RMSE_{log10(K)}$ and higher $R^2$ than the values predicted with the FXW-M1 model. This indicates that the physically estimated $K(h_m)$ in the dry range is a better representation of the matrix flow, while $K_m$ mostly reflects the impact of macroporosity (van Genuchten & Nielsen, 1985).

Additionally, the FXW-M2 model shows another advantage. The prediction of HCC is determined by the fitted parameters of SWRC. However, different combination of parameters may yield equally good fit between calculated and observed SWRC data, which, might yield different predictions of HCC. Equation 13 shows the new matching point $K(h_m)$ is fully determined by the value of water content $\theta_m$ and thus is not impact by the different combination of parameters, assuming they all give a close estimation of $\theta_m$. Therefore, including $K(h_m)$ as matching point provides an additionally physical constraint on the predictions of HCC.

However, except for sand soils, the FXW-M2 model with the default $l$ value of 3.50 tends to underestimate the conductivity, especially in the high water saturation range. The inflection point locates approximately at the observed conductivity of 0.01–0.1 cm d$^{-1}$, for which the corresponding matric potential is in the magnitude of negative tens of centimeters (Figures 6–10). When applying the optimal $l$ value for each soil type, although the FXW-M2-l model improves the prediction, it underestimates the conductivity near saturation, especially for fine-textured soils such as loam soils, silty loam soils, and silty clay soils (Figures 7–9).

The reason for the underestimation of conductivity near saturation for mainly fine-texture soils, as discussed in Schaap et al. (2001) and Schaap and Van Genuchten (2006), among many others, is that the water flow near saturation is impacted significantly by the presence of macropores or fractures. Schaap and Van Genuchten (2006) suggested an empirical value of −40 cm, above which the water flow is assumed to be impacted by macropores or fractures. This value is close to the critical value above which the FXW-M2 model tends to underestimate the conductivity (Figures 6–10).

Figure 11 shows the impact of macroporosity near saturation. As shown, the theoretically predicted $K_s$ with the FXW-M2 model is generally much smaller than the observed $K_s$ (Figures 11b–11d), confirming the effect of macroporosity near saturation. Treating $l$ as a free fitted parameter only slightly improves the estimation of $K_s$ (Figures 11d–11f), reflecting a limitation of the FXW series model in accounting for the impact of macroporosity. The original FXW model ($h_l = 0$) generally yields an overestimation of $K_s$ (Figure 11a). This is because the HCC in the FXW model drops dramatically for $n$ values close to 1.0, and a much higher $K_s$ is required to yield the estimated $K(h_m)$ in the dry range.

Therefore, to further improve the prediction of conductivity near saturation, the effect of macroporosity has to be considered. This, however, would introduce extra parameters, and is not considered in the current work.

In contrast to the obvious underestimation of conductivity near saturation for silty loam soils, and silty clay soils, it is interesting to note that for clay soils, the FXW-M2-l model generally shows a good agreement with observations (Figure 10). In this paper, the observed conductivity of the selected clay soils is generally less than 1 cm d$^{-1}$. That is, the impact of macroporosity is believed to be not important for the selected clay soils. While for silty loam and silty clay soils, the observed conductivity can be as higher as 100 cm d$^{-1}$ (Figures 8 and 9), reflecting clearly the presence of macropores. This might be the reason for the generally good performance of the FXW-M-1 model for clay soils.

5.3. Uncertainty From Data Observations

In this study, the applied data came from the UNSODA database. For most of the selected soil samples, the SWRC in the dry range was measured with the pressure plate method. However, as Bittelli and Flury (2009) argued, the pressure plate method tends to overestimate the water content for a matric potential of less than about
−2,000 cm. Since the estimation of the new matching point relies on accurate measurement of the water retention data in the dry range, the error coming from the measurement has an impact on the model performance. To evaluate this uncertainty, we present in Figure predictions of conductivity with different corrected water contents in the dry range. In Figure 12a, only water retention data higher than −2,000 cm is selected for fitting the SWRC, while in Figures 12b–12d, the water content measured for a matric potential less than −2,000 cm is multiplied by a correction factor. As shown, the prediction with the water retention data covering a potential higher than −2,000 cm yields a higher RMSE \( \log_{10}(K) \) of 0.93 cm d\(^{-1}\) (Figure 12a), compared to the 0.81 cm d\(^{-1}\) derived with the original UNSODA data (Figure 4c). For the predictions with different corrected water content measurements, a 50% reduction in measured water content for a matric potential of less than −2,000 cm yields a much poorer performance, with the \( \text{RMSE}_{\log_{10}(K)} \) being 0.96 cm d\(^{-1}\) (Figure 12d). The value, however, is still much less than the predictions with the FXW and the FXW-M1 models.

In Section 2, we showed that the estimated matching point \( K(h_m) \) shows a linear relationship with the measured/estimated water content \( \theta_m \) in the dry range. Thus, the impact of the observed water content data error on the conductivity prediction is much less than one order of magnitude. For the hydraulic conductivity, which can vary by several orders of magnitude, the impact from the measured water content error is thus not so great. In contrast, the shape of the SWRC has a much more dominant impact on the HCC (Figure 2). However, to accurately evaluate the performance of the proposed FXW-M2 model, reliable datasets are required. For example, the SWRC is measured by the chilled-mirror dew point devices in very dry conditions.

**Figure 11.** The predicted saturated conductivity with the FXW-M2 model for all the 159 soil samples. The impact of different values of \( h_s \) and \( l \) is represented in the different figures. The data density is represented by different color. The higher the value, the more samples are included.
5.4. Uncertainty in Estimating $K(h_m)$

The performance of the FXW-M2 model relies on accurate estimation of the matching point $K(h_m)$, which, in turn, is controlled by accurate estimation of the film thickness and the specific surface area. The determination of these two factors, however, can be impacted by many factors, such as the applied value of the Hamaker constant and the ionic concentration (Tokunaga, 2009, 2011). For example, Wang et al. (2017) discussed the impact of different Hamaker constant values, which are essentially different for different soil samples (Resurreccion et al., 2011; Tuller & Or, 2005), on the specific surface area and then on the film conductivity estimation. In addition, the possible water retained in very fine pores by the capillary force may also make a contribution to the conductivity, which, however, is neglected in estimating $K(h_m)$. Figures 4–10 show the FXW-M2 slightly underestimates the conductivity for most samples, therefore, a higher value of $K(h_m)$ than the estimation by Equation 13 can be expected to improve the prediction of hydraulic conductivity, especially for fine-textured soils. However, to further evaluate the possible impact of the referred uncertainty in estimating $K(h_m)$, there is an urgent need to establish a database that covers accurate measurement of hydraulic conductivity for different soil types in the dry range. Alternatively, in consideration of the difficulty in measured the HCC covering very dry conditions, we...
may apply the developed FXW-M2 model in modeling the soil evaporation process to test whether the default estimation of $K(h_m)$ can provide a good description of the evaporation process, which definitely covers water movement in very dry range.

6. Concluding Remarks

In this paper, we have proposed two modified forms of the soil hydraulic models developed by Fredlund and Xing (1994) and Wang et al. (2018), namely, the FXW-M1 model and the FXW-M2 model. The FXW-M1 model overcomes the abrupt drop of hydraulic conductivity near saturation for soils with small $n$ values. This is achieved by introducing a non-zero matric potential of $h_c$ following Vogel et al. (2000) and Ippisch et al. (2006), above which the water content was forced to be saturated. This slight modification improves the prediction of conductivity for soils with small $n$ values. A recent work by Wang et al., (2021) showed that, by applying this FXW-M1 model, the developed pedotransfer function, which predicts the soil hydraulic properties from easily measured soil texture information, improves the prediction considerably, compared with the original FXW model.

The FXW-M2 model provides a different way for predicting conductivity by applying an estimated conductivity in the dry range as the new matching point. Compared to the existing models that require the input of $K_s$, the FXW-M2 model can predict the HCC fully from the SWRC, without additional information. Because the new matching point that is estimated physically better reflects the matrix flow, while the observed $K_r$ is impacted by the presence of macroporosity, the new FXW-M2 model significantly improves the prediction of hydraulic conductivity. Therefore, it provides an easy and accurate way for predicting the HCC, which will facilitate water and solute transport simulation in land surface modeling.

However, the new FXW-M2 model does have one limitation, which is that it tends to underestimate the conductivity near saturation, especially for fine-textured soils. To address this shortcoming, the impact of macroporosity has to be considered in future work. Furthermore, a reliable database with accurate soil hydraulic measurements covering the dry range for different soil types is required to further improve the prediction of hydraulic conductivity when accounting for both capillary and adsorption forces.

However, to apply this method, the SWRC should cover measurements in the very dry range. When there are no direct observations, the water content at $h_m$ can still be predicted from the soil texture information. For example, several empirical relationships have been built between the clay fraction and the SWRC that accounts for the dry range (e.g., Arthur et al., 2013; Resurreccion et al., 2011; Schneider & Goss, 2012).

Data Availability Statement

The applied data were obtained from a public data set, which is available at the website of the United States Department of Agriculture (https://data.nal.usda.gov/search/type/dataset).
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