

Representation of the Influence of Soil Structure on Hydraulic Conductivity Prediction

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Abstract

The significant impact of soil structure on soil hydraulic properties and then on the associated water and solute transport is well recognized. However, existing soil hydraulic models that account for the effect of soil structure are often at the cost of overparameterization, hindering further application on large scales. In this study, we developed a new model that considers the effect of soil structure in hydraulic conductivity prediction when introducing no new free parameters. Testing with 152 soil samples that include different soil types shows that the new model considerably improves the prediction of conductivity, with an average root-mean-square-value (RMSE) of 0.65 cm d⁻¹. When applying the new model in fitting observations, the model showed excellent performance, with an RMSE of only 0.30 cm d⁻¹ remaining. This new soil hydraulic model provides a simple and practical way to incorporate the influence of soil structure in water and solute transport simulations.

1. Introduction

Soil structure, which refers to the arrangement of soil pore space (e.g., Rabot et al., 2018; Meurer et al., 2020), is an important property that is generally related to the effects of biological activity, abiotic factors or tillage practices. The significant influence of soil structure, such as the presence of macropores, on soil hydraulic functions, including the soil water retention curve (SWRC) and the hydraulic conductivity curve (HCC), and therefore on the associated water and solute transport has long been recognized (e.g., Dexter, 1988; Smettem et al., 1991; Zhang & van Genuchten, 1994; Durner, 1994; Mohanty et al., 1997; Nimmo, 1997; Šimůnek et al., 2003; Dexter et al., 2008; Jarvis, 2008; Beven & Germann., 1982; 2013; Jarvis et al., 2016; Vereecken et al., 2016; Robinson et al., 2019; Nimmo et al., 2021). Regarding soil hydraulic functions, early studies, such as van Genuchten and Nielsen (1985), Schaap and Leij (2000) and Schaap et al. (2001), confirmed that the application of the saturated hydraulic conductivity K_s as a matching point, which is sensitive to the presence of macropores, tends to considerably overestimate the unsaturated conductivity, which is mainly controlled by soil texture, especially for fine-textured soils.

To better describe the unsaturated conductivity, van Genuchten and Nielsen (1985) argued that the matching point should be taken at a point below saturation. Unsurprisingly, the prediction with the new matching point, however, will underestimate the conductivity near saturation. Othmer et al. (1991), Ross and Smettem (1993), Durner (1994), and many others further suggested that bimodal or multimodal soil hydraulic models should be applied to represent the influence of soil structure. For water and solute transport in soil, many studies have demonstrated the crucial role of macropores and have suggested that, instead of applying the classic Richardson-Richards equation, the dual-porosity or dual-permeability model should be used in regard to the impact of soil structure (e.g., van Genuchten & Wierenga, 1976; Germann, 1985; Gerke & van Genuchten, 1993; 1996; Jarvis, 1994; Šimůnek et al., 2003). The significant impact of the soil structure on the water cycle is also recognized for large-scale applications. For example, a recent study by Fatichi et al. (2020) showed that the inclusion of soil structure can considerably alter the infiltration-runoff process, especially in wet and vegetated regions. Bonetti et al. (2021) also demonstrated the crucial role of soil structure, which was further related to vegetation cover, in the infiltration-runoff process.

Despite the well-recognized importance of soil structure, representing the influence of soil structure is difficult and is often neglected in water and solute transport not only at the profile scale but also in the Earth System Model (ESM), which performs at regional to global scales (Fatichi et al., 2020). One main difficulty is that there is no simple soil hydraulic model that has the ability to capture the influence of soil structure without the cost of overparameterization. Although modified HCCs that account for macroporosity have been developed, such as Jarvis (1991), Børgesen et al. (2006), and Schaap and van Genuchten (2006), these modified models introduced a new parameter of the boundary hydraulic conductivity, above which the soil structure controls the water flow. This difficult-to-determine boundary conductivity therefore hampers the ability to predict HCC from SWRC, which is crucial for the practical application of soil hydraulic models. The bimodal or multimodal soil hydraulic models that were well established back to the early 1990s (e.g., Othmer et al., 1991, Ross & Smettem, 1993; Durner, 1994) do have predictive ability and consider the effect of soil structure. However, the developed dual-modal models introduce a large number of parameters. In general, the bimodal model has at least three more parameters compared to the commonly applied unimodal model, the most used van Genuchten (1980)-Mualem (1976) model for example. To determine the parameters, detailed measurements of soil hydraulic properties (in particular, near saturation) are further needed, which are often not available. The inclusion of too many parameters and the lack of measurements thus hinder the application of the existing bimodal hydraulic models, especially in large-scale applications.

The lack of a simple soil hydraulic model that accounts for the impact of soil structure also hampers the development of the pedotransfer function (PTF), which relates soil hydraulic parameters to more easily measured soil information, such as soil texture properties. ESMs rely heavily on PTFs to obtain the input

of soil hydraulic parameters for large-scale applications. However, few existing PTFs have been developed for bimodal soil hydraulic models that consider the effect of soil structure (e.g., Vereecken et al., 2010; Zhang & Schaap, 2017; Wang et al., 2022b). Additionally, it remains difficult to find easily measured indices or properties that can well represent the effect of soil structure (Díaz-Zorita et al., 2002). One well-demonstrated example is the relatively poor performance in predicting K_s from soil texture information with existing PTFs (Zhang & Schaap, 2017; 2019; Van Looy et al., 2017; Gupta et al., 2020).

Consequently, this study aimed to develop and evaluate a novel soil hydraulic model that considers the influence of soil structure. Specifically, we focused mainly on the impact of soil structure on HCC prediction, although it is evident that soil structure also impacts the SWRC. The reason for this is that water flow in macropores is often assumed to be driven mainly by gravity (Gerke, 2006), and the conductivity is of greater concern. Additionally, to describe the influence of soil macropores on the SWRC, a detailed measurement of water retention data near saturation and a large number of model parameters are needed. The developed new model has two properties: (1) it introduces no additional free parameters compared to the unimodal soil hydraulic model; and (2) it has the ability to predict HCC from the SWRC with the known matching point of K_s , as did the unimodal model. This study was motivated by a recent work by Wang et al. (2022a), where a simple and physically based model was developed that can predict the HCC fully from the SWRC without requiring the matching point of K_s .

2. Model Development

In this section, we first recall the FXW-M2 model developed in Wang et al. (2022a). Following this, we demonstrate the development of the new model that accounts for the effect of soil structure, termed the FXW-M3 model hereafter.

2.1. The FXW-M2 model developed in Wang et al. (2022a)

The FXW-M2 model developed in Wang et al. (2022a) has the ability to predict the HCC fully from the SWRC by introducing a matching point that can be estimated from the SWRC.

The SWRC of the FXW-M2 model is written as:

with $\Gamma(h_s)$ being:

In Equations (1) and (2), θ ($\text{L}^3 \text{ L}^{-3}$) is the volumetric water content and θ_s ($\text{L}^3 \text{ L}^{-3}$) is the saturated water content; h (L) is the matric potential; h_r is a shape parameter and is set to -1.5×10^3 cm, following Fredlund and Xing (1994); h_0 , which is set as -6.3×10^6 cm, according to Schneider and Goss (2012), is the matric potential corresponding to zero water content; h_s , set to -1 cm according to Wang et al. (2022a), is introduced to overcome the unrealistic decrease near saturation for fine-textured soils; and Γ (L^{-1}), n , and m are the fitted parameters.

The HCC of the FXW-M2 model is expressed as:

where h_m , set to -1.0×10^5 cm according to Wang et al. (2022a), is a typical matric potential where soil water is assumed to be in film form that is held solely by the van der Waals forces; $b(h_m)$, set to 2.693×10^{-6} cm d⁻¹, represents the combined effect of the estimation in film thickness, the specific surface area and the correction factor that results from the modified viscosity on conductivity prediction (Wang et al., 2022a). The detailed derivation of $b(h_m)$ can be found in Wang et al. (2022a). Equation (3) indicates that the HCC can be fully predicted from the SWRC, as all the parameters required are from Equation (1).

2.2. Accounting for the influence of soil structure—The FXW-M3 model

Although the FXW-M2 model matches the observations well in the medium to dry moisture range, it underestimates the conductivity near saturation for many soil samples (Wang et al., 2022a). This underestimation is attributed to the inability of the FXW-M2 model to account for the effect of macroporosity.

To represent the influence of the soil structure in the soil hydraulic model, the first step is to define a critical matric potential of h_a to distinguish the impact from the soil structure and soil texture. The corresponding hydraulic conductivity $K(h_a)$ can be estimated by Equation (3), written as

The maximum limit of K_s introduced in Equation (4) avoids the unrealistic estimation of the $K(h_a)$ value from the SWRC. For matric potentials less than h_a , the hydraulic conductivity can still be estimated by Equation (3). When the matric potential is higher than h_a , the impact of the soil structure becomes important. Here, we simply assume that the hydraulic conductivity for a potential higher than h_a can be described as a power function of the saturation degree S following Campbell (1974). The conductivity is written as

where n^* is a scaling factor.

As the conductivity $K(h_a)$ can also be estimated by Equation (5), the scaling Factor n^* can be described as

Resubstituting Equation (6) into Equation (5) gives the conductivity for matric potential higher than h_a , which is written as

Notably, for matric potential varying from h_a to 0, the saturation degree S is almost the same as $\Gamma(h)$ (Wang et al., 2016). Together with the conductivity described by Equation (3) for a potential less than h_a , the new HCC of the FXW-M3 model can thus be expressed as

Equation (8) has only one more parameter of h_a compared to the HCC of the unimodal soil hydraulic model. The value of the threshold potential h_a depends on the diameter of the smallest macropore of the individual soil. The reported h_a varies from approximately -4 cm in Børgesen et al. (2006) to -40 cm in Schaap and van Genuchten (2006). In this study, the exact value of h_a is determined by

optimizing the HCC with observations for a variety of soil samples. When h_a is determined, the HCC can be directly predicted from the SWRC with known K_s .

For the SWRC, Equation (1) can be applied. Alternatively, we can apply the SWRC developed originally by Fredlund and Xing (1994) for the FXW-M3 model. That is, the FXW-M3 model does not require the introduction of h_s as in the FXW-M1 model to overcome the unrealistic decrease in HCC for fine-textured soils (Wang et al., 2022a). The reason for this is that for matric potentials higher than h_a , a new conductivity function that has a fixed lower boundary of $K(h_a)$ is introduced in the FXW-M3 model (Equation 8). As a result, the HCC of the FXW-M3 model no longer showed an abrupt decrease for n values close to 1 (Figure 1). Consequently, we can apply the simple SWRC developed originally by Fredlund and Xing (1994) for the FXW-M3 model, which is written as

Equations (8) and (9) provide a simple way to describe the soil hydraulic properties from saturation to oven dryness. Both the impact of soil structure and soil texture are represented in the HCC. The bimodal shape of the HCC of the FXW-M3 model is clearly demonstrated in Figure 1. A higher potential of h_a and a smaller value of l represent a sharp decrease in hydraulic conductivity near saturation.

In contrast to other soil hydraulic models developed by Jarvis (1991), Børgesen et al. (2006), and Schaap and van Genuchten (2006) that deal with the influence of soil structure, the most pronounced advantage of the FXW-M3 model is that the boundary conductivity $K(h_a)$ can be fully determined from the known SWRC, while in other models, $K(h_a)$ has to be treated as a free-fitted parameter. As a result, the FXW-M3 model is able to predict HCC from SWRC with the known matching point of K_s . In addition, both the capillary and adsorption forces are considered in the FXW-M3 model, which enables a better description of soil hydraulic properties in the low water content range (e.g., Wang et al., 2016; 2018).

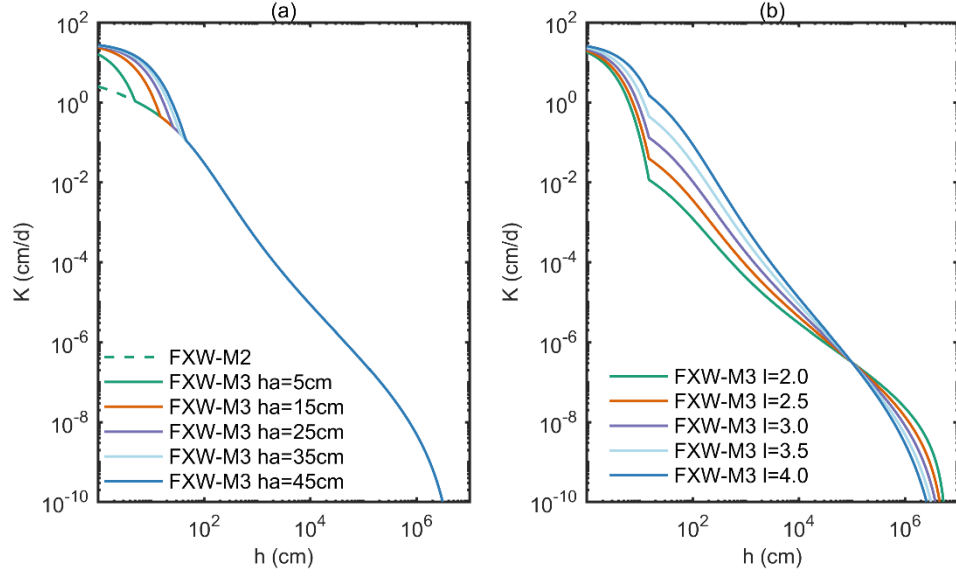


Figure 1. Illustration of the HCCs of the FXW-M3 model. (a) and (b) present the impact of different values of h_a and l on HCC prediction, respectively. The other parameters applied are $\theta_r = 0.02 \text{ cm}^{-1}$, $n = 1.01$, $m = 0.66$, $\theta_s = 0.45 \text{ cm}^3/\text{cm}^3$, and $K_s = 31.6 \text{ cm/d}$ for a loam soil.

3. Materials and Methods

3.1. Datasets

The applied datasets were the same as those applied in Wang et al. (2022a), except seven soil samples were omitted because the observed K_s is less than the unsaturated conductivity. As a result, a total of 152 soil samples selected from the UNSaturated SOil hydraulic database (UNSODA) (Nemes et al., 2001) were applied to evaluate the model performance.

3.2. Prediction of HCC

First, the optimal h_a was derived by fitting the HCC described in Equation (8) with conductivity observations, yielding an optimal h_a value of -28 cm (see Supporting Information).

Second, the SWRC described in Equation (9) was fitted with observations to derive the parameters. The objective function to be minimized is defined as:

where N is the number of water content observations and θ_i and $\hat{\theta}_i$ are the measured and fitted water contents, respectively. $p = (\theta_r, n, m, \theta_s)$ is the parameter vector used for the optimization. θ_s is only optimized when there is no observation. Equation (10) was optimized by applying the shuffled complex evolution method developed at the University of Arizona (SCE-UA), as proposed by Duan et al. (1992).

When the optimal h_a and the parameter vector p of the SWRC were determined, the HCC was then predicted by Equation (8) with the known matching point of K_s . For comparison, the FXW-M2 model proposed in Wang et al. (2022a) is also applied. Additionally, to demonstrate the flexibility of the FXW-M3 model in describing the HCC, we showed the fitted results by treating h_a and l as free-fitting parameters. The model was termed FXW-M3-Opt hereafter. All the optimized and fixed parameters of different model settings are listed in Table S1.

For each soil sample, the root-mean-square error ($RMSE_{\log 10(K)}$) and the coefficient of determination (R^2) are calculated to evaluate the model performance. The log-scale value is applied for conductivity.

The $RMSE_{\log 10(K)}$ is defined as:

R^2 is defined as:

where \bar{y} is the mean value of y .

4. Results

4.1. The overall performance in predicting HCC

The model performance for the evaluated 152 soil samples and for the six main soil types are summarized in Table 1. Compared to the FXW-M2 model, the FXW-M3 model with h_a fixed at the value of -28 cm substantially improves the prediction of HCC. For all 152 soil samples evaluated, the reported average $RMSE_{\log 10(K)}$ decreases from 0.73 cm d $^{-1}$ (the FXW-M2 model) to 0.65 cm d $^{-1}$ (the FXW-M3 model), while the reported average R^2 had the same value of 0.94 for the two models. When treating h_a and l as free-fitting parameters (the FXW-M3-Opt model), a reported average $RMSE_{\log 10(K)}$ of 0.30 cm d $^{-1}$ remains, and a higher average R^2 of 0.96 was achieved.

Table 1. Statistical values of different models for each soil type. The number in the bracket is the number of soil samples.

| Soil Type | Mean $RMSE_{\log 10(K)}$ (cm d $^{-1}$) | | Mean R^2 | | | |
|-----------------|--|--------|------------|--------|--------|------------|
| | FXW-M2 | FXW-M3 | FXW-M3-Opt | FXW-M2 | FXW-M3 | FXW-M3-Opt |
| Sand (28) | 0.70 | 0.65 | 0.40 | 0.95 | 0.96 | 0.96 |
| Sandy loam (23) | 0.79 | 0.63 | 0.33 | 0.93 | 0.93 | 0.93 |
| Loam (18) | 0.79 | 0.64 | 0.24 | 0.96 | 0.93 | 0.93 |
| Silt loam (40) | 0.62 | 0.50 | 0.25 | 0.91 | 0.94 | 0.94 |
| Silty clay (8) | 0.99 | 0.98 | 0.29 | 0.89 | 0.90 | 0.90 |
| Clay (10) | 0.70 | 0.68 | 0.32 | 0.94 | 0.96 | 0.96 |
| All (152) | 0.73 | 0.65 | 0.30 | 0.94 | 0.94 | 0.96 |

For the six main soil types, the improvement of the FXW-M3 model was more pronounced for sand, sandy loam, loam and silt loam soils, representing an

obvious decrease in the $RMSE_{\log10(K)}$ value (Table 1). For example, the FXW-M3 model reduced the average $RMSE_{\log10(K)}$ from 0.79 cm d⁻¹ of the FXW-M2 model to 0.63 cm d⁻¹ for sandy loam soils. For the R^2 value, both models showed similar values for different soil types. In regard to silty clay and clay soils, the FXW-M3 model only slightly improved the performance, with close $RMSE_{\log10(K)}$ values compared to the FXW-M2 model. When treating h_a and l as free-fitting parameters (the FXW-M3-Opt model), the model achieved a substantial improvement for all soil types, with reported $RMSE_{\log10(K)}$ ranging from 0.24 cm d⁻¹ (loam) to 0.40 cm d⁻¹ (sand).

4.2. Predicting HCC for individual soil samples

9 of 28 sandy soil samples, with a much lower $RMSE_{\log_{10}(K)}$ value compared to the FXW-M2 model (Figure 2a). For the other soils, both the FXW-M2 and FXW-M3 models have almost the same $RMSE_{\log_{10}(K)}$ value. The impact of soil structure is also shown in Figure 3 for two sandy soils, 2561 and 4660, where FXW-M3 considerably improves the prediction of conductivity near saturation. Additionally, a sharp decrease in water content is noticed near saturation (Figure 3).

Compared to the FXW-M2 model, the new FXW-M3 model improves the prediction of HCC for almost all 23 sandy loam soils, 18 loam soils and 40 silty loam soils (Figure 2b, c and d), clearly reflecting the impact of soil structure. Figure 3 shows that the FXW-M3 model achieves a better agreement with observations near saturation for the three loam type soils. Additionally, for some soils, such as 2590 and 2680, the SWRC does show a bimodal shape, which yet was not captured very well by FXW-M3. As a result, both the FXW-M2 and FXW-M3 models slightly underestimate the conductivity in the medium to low water content range. This underestimation occurs for most loam soils (Figure S5). In addition, for a few sandy loam samples, such as soils 2762, 2764, 4100, 4162 and 4172 (Figure S4), and silty loam samples, such as soils 2761, 4070, 4071, 4091, 4092 and 4182, the FXW-M3 model slightly overestimates the conductivity near saturation (Figure S6).

For the 8 silty clay soils, the FXW-M3 model has a similar performance to the FXW-M2 model (Figure 2e). The influence of soil structure is obvious for soils 1360 and 1361 shown in Figure 3 and for soils 1362 and 4680 shown in Figure S7, where the FXW-M3 model improved the prediction of conductivity near saturation compared to the FXW-M2 model. However, for almost all 8 silty clay soils, both the FXW-M2 and FXW-M3 models overestimated the conductivity in the medium to dry moisture range where matrix flow dominates, even though the fitted SWRCs of the two models are in close agreement with observations (Figures 3 and S7).

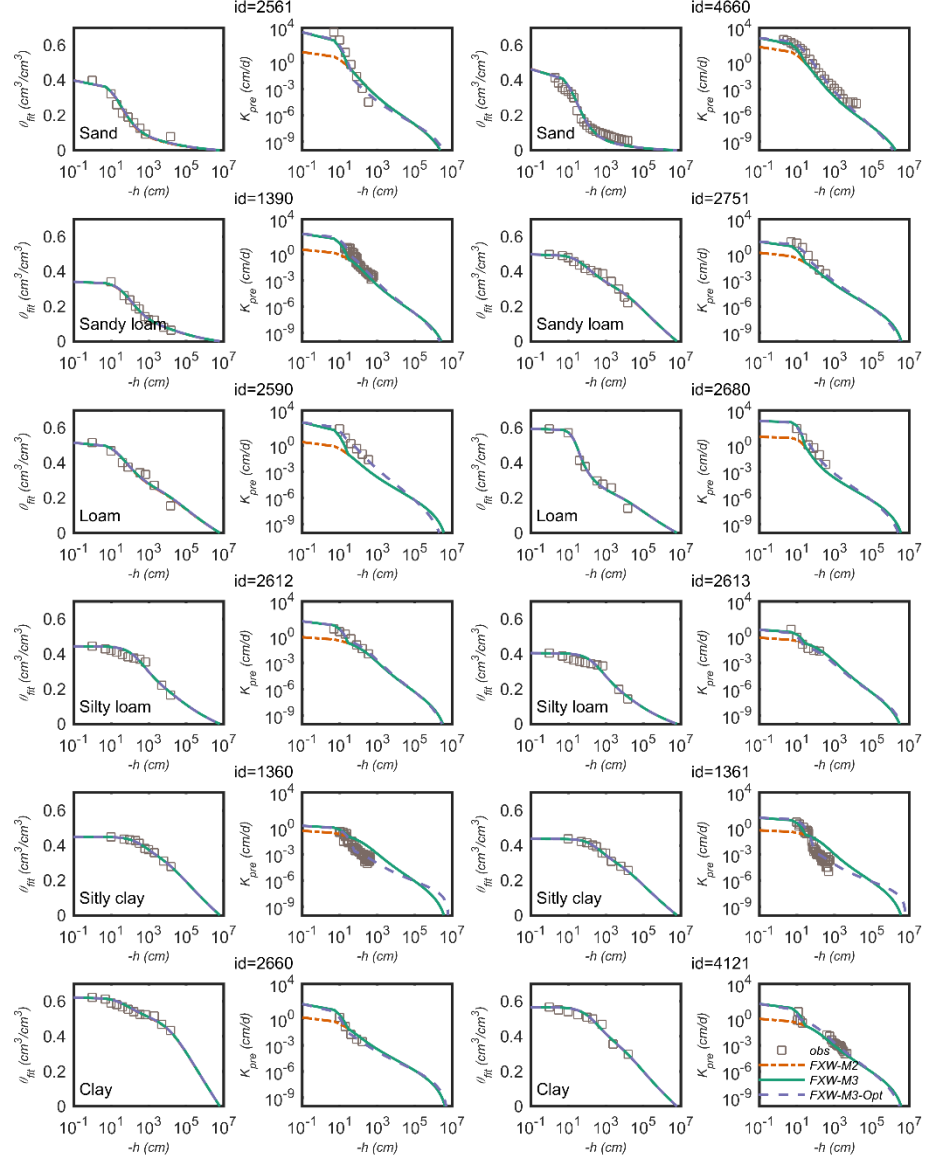


Figure 3. Predictions of the hydraulic conductivity with the FXW-M2, FXW-M3 and FXW-M3-Opt models. We show the results of two soil samples for each soil type. For each soil sample (represented by different IDs in the UNSODA

database), the figure on the left is the fitted SWRC, while the figure on the right is the predicted HCC.

The FXW-M3 model reported a lower $RMSE_{\log 10(K)}$ value for soils 2660, 4120, 4121 and 4681 (Figure 2f). The effect of soil structure, representing the bimodal shape of the SWRC and the underestimated conductivity of the FXW-M2 model near saturation, is also shown in Figures 3 and S8. However, only a few measurements were available for conductivity near saturation. For soils 2360, 2362 and 4121, both the FXW-M2 and FXW-M3 models tend to underestimate the conductivity slightly (Figure S8).

5. Discussion

In general, for the 152 evaluated soil samples that include different soil types, the proposed FXW-M3 considerably improves the prediction of conductivity compared to the FXW-M2 model developed in Wang et al. (2022a). The improvement, which also indicated the effect of soil structure, was more pronounced for sandy loam, loam, silt loam and, interestingly, also for sandy soils. For aggregated loam soils, the effect of soil structure is well recognized (Dexter et al., 2008). Sandy soils are usually assumed to be less impacted by the soil structure (Reynolds et al., 2009). The evidence from the HCC measurements and prediction indicates that the soil structure also has an important impact on some sandy soils. A further examination of soil texture information indicates that the impact of soil structure is important for sandy soils of low bulk density. For example, the bulk density is approximately 1.40 g cm^{-3} for soils 4140, 4141, 4660 and 4661. This suggests that the impact of soil structure is partially reflected in bulk density. In regard to silty clay and clay soils, the improvement to the FXW-M2 model was relatively small for the FXW-M3 model. This small improvement might be partially attributed to the small number of soil samples applied and few measurements near saturation available for evaluation.

When the FXW-M3 model was generally in close agreement with observations, it shows a slight overestimation of conductivity near saturation for a few soil samples. This overestimation was in part attributed to the uncaptured sharp decrease in water content near saturation by the SWRC of the FXW-M3 model (Figures S4-S8). According to Equation (5), the prediction of HCC relies on the accurate estimation of the saturation degree near saturation. A higher estimation of water saturation means a higher estimation of conductivity. In addition, this overestimation may also indicate that a higher h_a value than the fixed -28 cm should be applied for these soils. In this paper, the value of h_a is derived by optimization. Figure S1 indicates that the optimal value of h_a may vary among different soil types. When treating h_a and l as free-fitted parameters, the FXW-M3-Opt model considerably improves the estimation near saturation. The underestimation of conductivity in the medium to dry range for mainly loam soils is attributed to the uncaptured bimodal SWRC, as shown in Figures 3 and S4.

Both the FXW-M2 and FXW-M3 models tend to overestimate the conductivity

for silty clay soils in the medium to dry moisture range, although the fitted SWRC is in close agreement with observations (Figure S8). Wang et al. (2022a) showed that the estimated conductivity of the FXW-M2 model relies on the accurate estimation of soil water content at a matric potential of -1.0×10^5 cm, which is not yet covered by the measurements (Figure S8). The uncertainty that comes from the soil water content estimation in the very dry range might be the reason for the model overestimation. For clay-rich soils, in addition to the percentage of the clay fraction, the mineral type of clay also has a significant impact on the water content in the dry range (Lehmann et al., 2021).

The deviation in HCC prediction that comes from the uncaptured SWRC indicates that to fully describe the influence of soil structure, the bimodal SWRC should also be applied in addition to modifying the HCC. However, as discussed in the introduction section, the application of the bimodal or multimodal SWRC introduces too many parameters and requires a detailed measurement of water retention data (e.g., Othmer et al., 1991, Ross & Smettem, 1993; Durner, 1994). This complex bimodal soil hydraulic model may be useful in profile applications but is impractical in large-scale applications.

6. Concluding remarks

In this study, we developed a novel model for HCC prediction by considering the effect of soil structure. In comparison with existing models that account for the impact of soil structure, such as Durner (1994), Jarvis (1991), Børgesen et al. (2006), and Schaap and van Genuchten (2006), this new model has no cost of overparameterization and is able to predict HCC from SWRC with the known K_s . In addition, the new FXW-M3 model accounted for both the impact of capillary and adsorption forces and yields a much better description of soil hydraulic properties in the low moisture range compared to the commonly applied capillary-based models (Wang et al., 2016). Therefore, the FXW-M3 model accounts for both the impact of soil structure and soil texture and is able to describe the soil hydraulic properties from saturation to oven dryness when introducing no additional free parameters compared to the well-known van Genuchten (1980)-Mualem (1976) model.

This new FXW-M3 model provides an easy and practical way to incorporate the influence of soil structure in water and solute transport simulations. It also enables the development of new PTFs that account for the impact of soil structure, which is crucial to represent soil structure impact in ESM models. However, this study only represents a first step to account for the influence of soil structure in water and solute transport processes. To fully capture the influence of soil structure, we need to build a new soil water flow equation than the classic Richardson-Richards equation and to find an easily measured/accessed index to represent the effect of soil structure and to further develop new PTFs, which is crucial to represent the influence of soil structure in large-scale applications.

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(<https://data.nal.usda.gov/dataset/unsoda-20-unsaturated-soil-hydraulic-database-database-and-program-indirect-methods-estimating-unsaturated-hydraulic-properties>).

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