

Dear Editor,

„All models are wrong, but some are useful“ (Box, 1976).

We may preface this response by saying that we are surprised at both the fundamentality of the content of the criticism of our work and also the somewhat disparaging style of the review. With his text, the anonymous reviewer questions the foundations of soil hydrology and discredits most of the past work in this field on the basis of fundamental considerations. That's fair, but the scientific dispute should remain constructive, no matter how different basic views are.

It is known for long that estimating soil hydraulic conductivity from the water retention curve as a model of the pore size distribution with concepts that are based on bundles of capillary tubes has fundamental limitations. Accordingly, it has been strongly criticized (e.g., Hunt et al, 2013). Nonetheless, such approaches are currently and foreseeably will continue to be the backbone of parameterizations of SHP for practical application. The reason for this is probably not the stubbornness of old-school soil physicists, but simply the fact that the method is useful (as shown in our work), while proposed alternatives have so far proved to be unavailing.

Our study contributes to the general question of how close predictions of the capillary part of the HCC come to measured data, using some of the most prominent capillary bundle concepts that are established in historic soil hydrology. In doing that, it contributes to science by adding a piece of knowledge. In our view, the study is sound, since we clearly state what we want to do, which methodology we use, and how we come to results and conclusions.

To question this on the basis of fundamentally different views is, in our view, misplaced, since the same reasoning can be used to question any other useful modeling, such as the use of the Richards equation or the advection-dispersion equation in soil hydrology. Our view is that this would be inappropriate as long as superior approaches are not established.

Kind regards,

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In the following we will give a point-to-point reply to the comments of reviewer #2.

Major comments

The approach advanced here by the authors (and in previous publications) rests on pragmatic arguments for representing the complexity of WRC and HCC which considerable number of ad-hoc approximations and parameters. This is not meant to judge such efforts as “useless” – these effects have their practical value and place as long as authors and readers remember these are simplifications made for practical applications by Peters and Durner (2008 and the string of studies thereafter) and should not be confused with physically-based theoretical frameworks – while the so-called PDI model contains several physically based elements, it is also riddled with empiricism that makes the title read a bit overstated. Moreover, in contrast with the calibrated language of Peters et al. (2021, WRR) statements are now made as if the simplifications made over the years are now “facts”.

It is undoubted that our HCC prediction model is semi-empirical, and we are sorry if our recent work gave the reviewer the impression that we are claiming it to be entirely physical. However, in the recent two papers (Peters et al., 2021; 2023), we put more and more physical knowledge into the model in

order to extrapolate if insufficient information is available (i) in the dry (Peters et al., 2021) and/or (ii) in the wet range (Peters et al., 2023). We will take this statement by the reviewer as an argument to go through the text carefully and make it clearer that our model contains empirical elements.

Notably, our title does not contain any statement of “physics based” or similar. For us, “full prediction of HCC” simply means that we predict HCC without conductivity data, and this is the case after we calibrate the model. However, if this notation might be misunderstood as pure physically prediction we therefore will slightly change the title to “Prediction of absolute hydraulic conductivity—comparison of four different capillary bundle models”

Various important assertions are made with no basis, such as: “representing the soil hydraulic properties in functional form is mandatory for simulation of water...” this simply not correct – many numerical models have been doing fine with lookup tables and other data-based information. The use of parametric models is a mere computational convenience as these models contain no new information (about SHP) other than what is contained in the data used to estimate parameters.

We fully agree. We will replace “mandatory” by “useful”. The main reason for using functional representations of SHP’s is that measured data are usually limited. In many cases, neither do we have data in the dry range for both functions, nor do we have conductivity data close to saturation. In such cases, which are the rule rather than the exception, we must extrapolate. Furthermore, bridging large data gaps requires interpolation. In such cases, having the functional form is maybe not mandatory but of great advantage. Moreover, measured data contain errors. Interpolating between noisy data points cannot lead to reasonable descriptions of transport properties. This is most clear for the derivative of the water retention curve, the water capacity function.

Many of the authors' pragmatic applications and approximations are useful, however, these need to be constantly stated to avoid confusion – my primary concern with this work is with the hyped representation of what is essentially an empirical model as theoretically-derived and physically-based. The cutoff critical pressures for non-capillary water, the arbitrary interpolation of the WRC to the dry end; the basis for the hypothesis of a universal tortuosity scaling coefficient; even the fact that eq. 22 in Peters et al. 2023 showing proportionality of K_s with α^2 has not been tested with hard data... Until “predictions” are made for unknown soils and broadly tested I would refrain from using terms such as “full prediction of unsaturated hydraulic conductivity (function)...”. I don’t want to belittle the hard work of the authors, however, such a proclamation in the title sounds more like a mantra at this stage.

This comment refers to already published work and not to the recent manuscript. We disagree that our recent version (Peters et al., 2021; 2023) is purely empirical. It contains empirical elements but the extrapolation of the HCC in the dry range is a simplified form of the model of Lebeau and Konrad (2010), which is based on the theoretical works of Tuller and Or (2005) and Tokunaga (2009). From our point of view, the invoked simplifications are justified by the analysis given in Peters et al. (2021) (e.g. Fig. 2). The prediction of the capillary part is indeed more empirical and this is stated in Peters et al. (2023) and intrinsically in this manuscript because we calibrate the models to data. Even in the introduction of this manuscript we do not claim that the prediction of capillary conductivity is pure physics. However, this approach contains more physical elements than the classical models, where the measured saturated or unsaturated conductivity is used to scale the relative conductivity function for each specific soil sample.

With respect to the exact “cutoff critical pressures for non-capillary water”: yes, it is not based on basic physical consideration, but for the purpose of the model it is not important, since the WRC and the HCC are dominated by capillary water at this pressure range.

Referring to the critique about the interpolation of the WRC to the dry end: this is not arbitrary. It is empirical, but it is based on experimental data, which go back to the work of Campbell and Shiozawa (1992). The almost linear course in the semilog plot is found in several data sets, which are nowadays regularly obtained by the dewpoint method. However, we agree that there is no strong physical basis for this course. But we do not claim this in any of our papers.

The basis for the hypothesis of a universal saturated tortuosity scaling coefficient goes back to the early work of Carman (1937). Our empirical approach that uses the saturated tortuosity coefficient as a parameter that lumps not only the path elongation due to tortuosity but also other effects is clearly stated in Peters et al. (2023). For convenience, we literally quote this here:

“In real soils, however, the deviation from flow in straight capillary bundles is not only affected by tortuosity in the strict sense but also by other soil-related factors such as the surface roughness of pore walls, non-circular capillaries, and dead-end pores. Additionally, not only the geometry of the pore space may differ from the ideal case but also such fluid properties as surface tension and viscosity likely will be different from those of pure free water. Finally, capillary bundle models will not represent the pore distribution and connectivity in an ideal way. Therefore, we seek in this contribution an empirical value of τ_s that lumps all these effects. The hypothesis that τ_s varies only moderately among different textures will be tested by fitting predicted K functions to test data.” (Peters et al., 2023, section 2.3).

The fact that eq. 22 in Peters et al. (2023) shows proportionality of K_s with α^2 is given by the mathematical derivation under the assumption that a general value for τ_s exists. Furthermore, it is simple physics and can also be derived by the Hagen-Poiseuille law, because α scales the suction, the suction is inversely proportional to pore radius and conductivity is proportional to the square of the pore radius.

As a reaction on the reviewer’s critique, we will change the title of the paper as indicated in the reply to the first major comment.

In the following I make a few observations to place this work in context:

1. K_v (vapor transport) is not and should never become a component of the HYDRAULIC conductivity function. While capillary and film flow components obey viscous flow (liquid under shear), K_v emerges from and obeys Fick’s law of diffusion... I found referencing to Saito et al (2006) insufficient to resolving this fundamental physical discrepancy. Like many others, the reviewer fully understands the dilemma of HCC representation at the dry end, yet I would stay away from mixing two different physical transport processes by using the same function even for the sake of practicality (calling it $K_{\text{effective}}$ is not helping much).

As a first remark, K_v does not play a role *in this specific manuscript* as it deals with the comparison of different capillary bundle models, i.e., it focuses on differences in the wet moisture range where capillarity dominates. However, as derived by Saito et al. (2006), Fick’s law of vapor diffusion can be directly translated into potential theory, and under isothermal conditions (and only then), we can incorporate K_v into the HCC. It makes practically no difference if liquid and vapor flow are summed up in the flow equation or already in the HCC if the impact of the gravitational potential gradient is much smaller than the suction gradient, which is warranted when water flow takes place under very dry conditions (see Peters, 2013, Vanderborght et al., 2017; Iden et al., 2021a,b). We note, however, that such simplifications must be treated with caution and be avoided if solute transport is simulated.

2. In general, I found the motivation for the present study to be poorly defined. While the authors have been motivating their refinements of already existing models under the “umbrella” of pragmatism, how is comparing 4 or even 10 fundamentally flawed bundle of capillaries (BCC) models advancing the field? None of these models ever claimed to represent real soils, they do not consider film flow and cannot possibly address issues of liquid topology and connectivity other than via some ad-hoc tortuosity factor. So, whether a certain approach scales then normalizes or vice versa makes no difference in the fundamental fact that these are very poor toy approximations.

We think we have already made our motivation very clear in the abstract:

“While various expressions for the WRC are commonly compared, the capillary conductivity model proposed by Mualem (1976a) is widely used but rarely compared to alternatives. The objective of this study was to compare four different capillary bundle models in terms of their ability to accurately predict the HCC without scaling the conductivity function by a measured conductivity value.”

About the selected models: it is absolutely true that such capillary bundle models are crude simplifications given the complexity of real soils. We believe this is well known in the scientific community, but in the revised manuscript, we will make this even clearer. Yet, due to their practicability, the capillary bundle models are often used and they were developed to represent hydraulic conductivity in real soils. For our comparison, we identified those capillary bundle models which are cited the most often, which are simple to implement, and which are accordingly most often used in practice. We will make this reasoning clearer in the revised version. Of course, other researchers are invited to use other models and other data.

3. To be specific regarding the motivation, the authors state in the abstract "The objective of this study was to compare four different capillary models in terms of their ability to accurately predict the HCC without scaling the conductivity function by a measured conductivity value". Upon reading this very specific objective it reads arbitrary and contrived (almost as it has been formulated after the study was completed...). Given the nature of these BCC models - how is comparing different BCC models with numerous parameters, thresholds and simplifying assumptions addresses the overall goals of the opening statements? (reliable data, accurate information, and SHP models). I am also puzzled by the notion of "accurately" - measured how? Is this the Akaike information criteria (Peters et al. 2021) is this proximity to a set of incomplete measurements as shown in the supporting materials? The point is that these models have been proposed and are used because they capture salient features of the capillary retention and (with many additional assumptions) also capillary flow processes. Devising another ad hoc set of parameters is not likely to lead to new insights or advance the field. I was able to count at least 20 parameters (from several pressure threshold criteria, to extrapolation schemes for WRC dry end and HCC, to smoothing parameters, and so on). I am thus left confused and wondering if the authors seriously consider these nuanced additions to be of practical use for say, watershed hydrologic models or Earth system modeling? or even for predicting solute transport in their own backyards?

Our semi-empirical model for predicting hydraulic conductivity (Peters et al., 2023) was based on the model of Mualem (1976). Of course, and this is the purpose of this manuscript, we were subsequently curious if and how the prediction accuracy could be affected by different conceptualizations of the capillary bundle models (all of which are wrong but have proven useful in the past). As indicated in the reply to the previous comment, we chose the 4 selected models, because the Burdine and the Alexander and Skaggs models are often cited together

with the Mualem model, which has become the standard model. We further regarded the CCG model as a seminal contribution to this field of soil physics, which was the basis for the derivation of the Mualem model.

With respect to the question *“how is comparing different BCC models with numerous parameters, thresholds and simplifying assumptions addresses the overall goals of the opening statements?”*, we stated in the title, the abstract, and in the methods section that we use these models for prediction. The “numerous” parameters belong to the model structure, not prediction. Actually, a user that applies this model needs only to fit the retention model to the data and gets a prediction of the HCC without the necessity to adjust any additional parameter.

With respect to the question *“accurately - measured how”*: “Accurate” means unbiased and with small variance. This is quantified by the RMSE and this is written in the manuscript and shown in several box plots and displayed in the plots showing the predicted HCCs.

“Devising another ad hoc set of parameters is not likely to lead to new insights or advance the field.”: We disagree. The question of the paper was to check whether use of alternative pore bundle based capillary conductivity prediction models, as compared to the factual reference model of Mualem (1976), will lead in the framework of the model of Peters et al. (2023) different prediction accuracies. The study showed that there are slight differences, and within the range of the selected model alternatives the use of Mualem’s model is still the best choice. To our understanding, this is an additional piece of knowledge that is worth to be communicated.

4. While there is nothing wrong with the mathematics, nor with various decisions made by the authors such as: saturation of 0.75 is a reasonable threshold for the end of capillarity and the onset of adsorption - the question I am grappling with is how this exercise in mathematical parameterization will advance our science? **Wouldn’t any machine learning algorithm outperform all these assumptions if “accurately” is defined as in Peters et al., 2021?** I wish the authors would have elaborated more on the innovation, novelty, generalization, etc. (declaring a new tortuosity factor “universal” is not enough – it needs to be shown).

Again, this statement of the reviewer refers to the already published papers of Peters et al. (2021; 2023). In the current manuscript, we simply compare four conceptually different capillary-bundle models and test their prediction performance with the 23 test data sets. Of course, other researchers are invited to conduct independent tests or develop alternative prediction schemes based on machine-learning algorithms.

With respect to *“saturation of 0.75 is a reasonable threshold for the end of capillarity and the onset of adsorption”*: We are afraid the reviewer misunderstood our model. Both parts (capillary and non-capillary) overlap in the whole suction range and both are forced to $S = 0$ at oven dryness.

5. To properly review this study, I had to look back into a string of publications from the same authors. It is probably unintentional, however, when these studies are read in a sequence, one can notice the gradual “erosion” of qualifying statements that appeared in early work with some of the assumptions are now presented as established “facts” referring to previous publications (I much preferred the calibrated language of Peters et al. 2021; WRR). Perhaps a section on assumptions and approximations can help readers navigate through the physical and empirical elements of the study.

We are thankful for this hint and will go carefully through the manuscript to state the “*gradually disappearing qualifying statements*” about the underlying model assumptions more explicitly.

6. Even the choice of using the capillary part of the WRC to deduce capillary flow under the HCC lacks depth – how the authors envision different liquid configurations in the pore spaces, liquid topology, continuity etc. – all of which must affect the “Full prediction of unsaturated HCC”

Again, this refers to the already published paper of Peters et al. (2023). A “full prediction of the HCC” is done (to our definition) if no parameter of the HCC must be calibrated by a user that applies the model. The different liquid configurations in the pore spaces, liquid topology, continuity etc. are all lumped in the empirical capillary bundle model with the parameter τ_s . This is of course daring and we cannot expect that it is able to represent all the differences of pore-scale configurations of different soils; However, this is always done if capillary bundle models are used to describe the HCC, also if the relative HCC is scaled by a measured value, and we were pleased to find out that the full prediction seems to work amazingly well as shown in the present study.

To explicitly account for different liquid configurations in the pore spaces would require information of additional characteristics for any specific soil or other simplifying assumptions about the pore geometry have to be made (as done e.g. by Tuller and Or, 2001). The crucial point is that one must always make simplifying assumptions regarding pore geometry in the framework of continuum theory.

7. Other than lip service to the role of film flow in the unsaturated HCC – not much is presented here to support a “Full prediction”. Can one use characteristic “grain diameter” as a substitute for surface area as in Kozeny-Carman or even Lebeu and Konrad – of course, not.

Again, this comment refers to previous published work. Peters et al. (2021) showed that we use a simplified version of the Lebeu and Konrad (2010) model to predict the “film flow” part of the HCC. The parameter c in Equation A.6 of this current manuscript lumps all the physical constants as well as characteristic grain diameter (which is in accordance to Lebeau and Konrad derived from the water content at $h = 10^3$ m). We refer to section “2.2.2.Calculation of Absolute Non-Capillary Conductivity From the Water Retention Curve” in Peters et al. (2021).

There are hundreds of papers in the geophysical literature that show the failure of such approximation in shaly formations (clay soils). Where is the key parameter of soil specific surface area responsible for most of the films in the dry end of the WRC – this is part of my skepticism of the physical basis of the derivations here. Until WRC models embrace this critical (physical) parameter affecting many soil processes, there will always remain a representation gap of adsorption processes. No amount of BCC representation and tortuosity acrobatics is likely to fill in this gap!

We appreciate this comment and agree that soil specific surface area might be a critical parameter specifically in clay soils (which anyhow pose huge problems in the context of SHP models that assume rigid pore systems). Clearly, a test of the usefulness of our model for the addressed soils would be very interesting and we are happy if researchers who have access to such data will do this. We note however, that this is not referring specifically to the purpose of this paper, the comparison of four semi-empirical capillary conductivity models.

I have other specific comments regarding presentation (similar colors of lines with no legends), and how inferences were made (how performance was measured), however, these are minor points. I am

debating between recommending a major revision and an outright rejection of the manuscript until the key issues above are resolved – in any case, the decision rests with the editor.

We would have appreciated receiving specific comments to improve our manuscript in order to achieve the clearest possible presentation of the content.

Regarding the general evaluation of the work, we reiterate that the negative comments are of a fundamental nature and relate mainly to previously published work by our group and the use of capillary bundle models in general. We believe that a discussion by the anonymous reviewer of this issue and its publication in HESS as separate opinion paper would be most appropriate.

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