Dear Editor,

Please find a point-to-point reply to “RC3: 'Reply on AC2', Anonymous Referee #2, 15 Jul 2023”, regarding the discussion of preprint hess-2023-134. The reviewer’s comments are repeated in black font, our replies are set in blue font.

Kind regards,
Andre Peters, Sascha C. Iden, and Wolfgang Durner

Major comments

1. It is unlikely that the authors would retract inaccurate assertions made in previous publications such as, that the use of parametric models is “mandatory” (see introduction in Peters et al. 2023), their recurring argument that because certain information has been published previously precludes it from further scrutiny (in this review) is inconsistent. Not only because of the permanently tentative basis of the scientific method, but also considering potential confusion of young students exposed to such assertions without knowledge of the broader picture.

   In our initial response, we emphasized the potential benefits of parametric models, as they can be very valuable in practical modeling. We welcome open discussions about this topic, as well as other related issues. Scientific progress thrives on debate and differing viewpoints. However, we believe that the current review process may not be the most appropriate platform for a comprehensive discussion of such matters. Instead, we encourage the reviewer to write an independent opinion paper in which he/she expresses his/her criticism of our work and the efforts of others to develop soil hydraulic models for both scientific and practical applications.

2. Considering that each equation and statement you are making in this work is subject to scrutiny, the authors can choose among several options. If vapor transport or film flow are NOT part of the proposed theory (which they shouldn’t as non-capillary components of the representation), the right thing to do is (1) to disclose these limitations upfront (hence, “full prediction” is properly qualified) and/or (2) not repeat these derivations here and treat these as “facts”.

   From the ongoing discussion, it became evident that the term "full prediction" may not accurately convey our intended meaning. What we truly meant to express is the concept of a "pure prediction", emphasizing that we solely rely on the water retention curve's information and abstain from incorporating any measured hydraulic conductivity data into the derivation of the corresponding function. We furthermore refer to our reply to point 4, below.

   Concerning the incorporation of film and vapor conductivity in the HCC prediction, it is imperative for us to incorporate at least the film conductivity in our present study. This comes from the fact that the majority of utilized datasets cover both, the capillary and the film-dominated range. Additionally, we find no significant practical obstacles in utilizing either the film conductivity prediction proposed by Peters et al. (2021) or the isothermal vapor conductivity prediction derived from the research conducted by Saito et al. (2006).

   By presenting derivations, we aim to clarify that they are not presented as absolute facts, but rather as a means for readers to comprehend and trace the foundations and assumptions of our models. Therefore, we find no reason to exclude these derivations or references to the models we utilized, as they contribute to transparency and understanding for any interested reader.

3. For context – I have not seen a fundamental explanation for why Kv (vapor transport component of K) should be lumped with the HCC. This perpetual misconception was mentioned again here (A.5) and commented that "Kv as a function of the invoked WRC" (how is this exactly a function of the WRC – via eqs. 12 and 13 in Saito et al. 2006?). If there is a sense of "somewhat disparaging style of the review" it is probably my subconscious response to the shockingly sloppy science that places the burden of proof for such blunder on a numerical study by Saito et al. 2006 (attempting to solve the Richards equation with vapor transport) – I give the authors more credit than reflected in this off-hand response and reference to Saito et al. 2006. Not only that this is categorically not hydraulic conductivity and cannot be linked with coefficients that describe shear flow of liquid in proportion to pressure gradients (or potentials); the underlying gradient of potential energy that drives flow of liquids in porous media is not the proper gradient for vapor transport as discussed (many years ago) by: L. Monteith, G.S. Campbell, 1980, Diffusion of water vapour through integuments—Potential confusion, Journal of Thermal Biology, 5(1) 7-9 "The appropriate potential is the concentration of water vapour in air or the vapour pressure. The free energy of water is not an appropriate potential and Toolson's (1978) analysis for arthropods is therefore incorrect". I hope the authors would take this into consideration and refrain from lumping these different processes into the HCC.

We start with the "fundamental explanation for why Kv should be lumped with the HCC". Clearly, diffusion of water vapor in porous media is described by Fick's law. The water vapor pressure in the soil is the product of the saturation vapor pressure, which depends on temperature only, and relative humidity, which is a function of the water potential. The basic reasoning can be found in Philip and de Vries (1957), Nassar and Horton (1989), Noborio et al. (1996); Fayer (2000) and Saito et al. (2006). In the article by Saito et al. (2006), the only relevant equation is Eq. (12), while Eq. (13) describing thermal vapor conductivity is irrelevant for our analysis. The relationship with the WRC becomes obvious in Eqs. (14) and (15) in Saito et al. (2006) which define the dependence of the diffusion coefficient for water vapor in the soil on soil water content. What remains is the question why one can lump the vapor conductivity Kv with the liquid conductivity Kliq. Actually, this lumping is not described in Saito, but justification is given in Peters (2013) and Iden et al. (2021). Adding the two conductivities is only possible if the gradient in matric potential is much higher than the gradient in gravitational potential. This is the case under evaporation conditions. So yes, the lumping is based on pragmatism. The question whether the Richards equation can only be applied to "shear flow of liquid in proportion to pressure gradients" as stated by the reviewer is an interesting one. From our point of view, the Richards equation (RE) is a partial differential equation which should be judged by its potential to describe flow processes. Evaporation from dry soil necessitates the inclusion of vapor flow and therefore adding Kv to Kliq is required to adequately describe water flow in soil with the RE. Anyway, the issue of lumping vapor flow with liquid flow is certainly not important for the presented comparison of capillary bundle models as these deal exclusively with the capillary part of Kliq. One must keep in made, however, that the combined flux of liquid and vapor water cannot serve as the base for solute transport under dry conditions. As an illustration, in Peters et al. (2019), we separately calculated water transport in the liquid and vapor phases, specifically addressing the "back-dispersion" problem.

4. Finally, for perspective – (i) the authors' claim of "full prediction of HCC" – but also argue that "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". In physics, "full prediction" implies generality afforded by physical principles otherwise we correlate, calibrate, estimate etc.; (ii) it would have been appropriate to mention the pioneering study of: Jackson, R.D., 1972. On the calculation of hydraulic conductivity. Soil Sci. Soc. Am. Proc. 36:380-383. (and an earlier study by Jackson et al., 1965, WRR very similar to this one – both have been cited by van Genuchten 1980). Jackson 1972 was published over half a century ago and uses similar line of reasoning and tools as the authors are reporting here (and in Peters et al. 2023) to "fully" predict the unsaturated hydraulic conductivity function. What remains from this early effort are: (1) the motivation of van Genuchten 1980 and others to convert WRC to HCC; and (2) a nice classroom exercise regarding how this might work using the BCC usually accompanied with a stern warning that there is no predictability power here simply because liquid organization (the capillary flow pathways) are NOT representable in this lumping exercise. Fifty years later, the authors are claiming to have solved the problem – yet other than curve fitting (not that different from Jackson et al. 1965, WRR) there is no fundamental physical explanation of how this magical tortuosity factor works and how general is it.

Again, we are a bit irritated by the fundamental nature of this criticism, which amounts to a general reckoning with existing practices in soil hydrology. In the field of physics, the wording "full prediction" might indeed imply generality afforded by physical principles. However, we employ the term "prediction" in its conventional context, which refers to the process of calculating a HCC (Hydraulic Conductivity Curve) from the WRC (Water Retention Curve) using capillary bundle models. This usage of "prediction" has been a common practice in soil hydrology since the early adoption of these models, as evidenced by its inclusion in literature such as Mualem's "Methods of Soil Analysis" (1986). Notably, van Genuchten's seminal work from 1980 also employs "prediction" in its title.

We do not perceive it as our responsibility to replace this established terminology with an alternative that may be more theoretically accurate. As a compromise, we will modify the title and corresponding sections of the text to refer to "prediction of absolute conductivity," as previously mentioned in our initial response. This adjustment will better reflect the intended concept without deviating significantly from the commonly accepted terminology in the field of soil hydrology. "Correlate, calibrate or estimate" are certainly not the right verbs in this context.

We are thankful for hinting to the two references of Jackson and co-workers and will mention them in the introduction section. However, the claim that we do the same exercise as Jackson is wrong. Jackson (1972) compared two capillary conductivity models and predicted the <u>relative</u> conductivity and scaled it with a measured matching factor (saturated conductivity). Seven years earlier, Jackson et al. (1965) compared 4 models and either predicted the absolute hydraulic conductivity or used one matching factor. In their work, the absolute prediction overestimated the conductivity drastically. In contrast, we calibrate a general saturated tortuosity factor (not "magical" – see Peters et al. (2023) section 2.3 "Absolute hydraulic conductivity prediction") and use it to predict the absolute conductivity for independent data sets. With the appropriate retention model and conductivity models it works quite well with a median RMSE_log10(K) of 0.4. Certainly, it is not perfect but, to our point of view, much better than previous attempts. We emphasize that our suggestion to predict the absolute conductivity is meant to be used to overcome problems in cases in which sufficient data is NOT available for a certain soil.

Finally, we wish to address a potential misunderstanding regarding our work. Our objective is not centered around enhancing the comprehension of mechanistic modeling concerning the intricate physics of fluid mechanics in unsaturated heterogeneous porous media. Instead, we focus on utilizing and streamlining established physics to derive practical models that reduce systematic errors in comparison to alternative existing models. Ultimately, the effectiveness of our approach will be evaluated by comparing the predictions of the HCC with measured values by other researchers. We eagerly anticipate such comparisons as they will provide valuable insights into the performance and reliability of our models.

Since most of the raised points of the reviewer are concerned with our and other's previous work and also with the use of capillary bundle models in general, we repeat our suggestion to write an opinion paper.

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