Sigmoidal Water Retention Function with Improved Behavior in Dry and Wet Soils HESS 2020-380

Reply to referee 2

The text by the referee is in *blue and italics*. Our response is in black and regular font.

Referee report

GENERAL COMMENTS The standard parameterization of soil hydraulic functions that is used in the modeling of unsaturated water flow may imply 'non-physical' behavior for certain parameter combinations (i.e. soil types). The authors propose a new approach with better description of the processes under very dry and very wet conditions. Based on numerical experiments, the authors could show that the simulations using the new proposed hydraulic functions were more stable compared to other parameterizations (simulations could be completed for more scenarios with fine textured soils). The discussion of the limits of the standard approach is important to ensure that it is not applied in an uncritical way. In addition, the parameterization of hydraulic functions allowing stable simulations for a wide range of soil types and conditions is relevant. Hence, the motivation and objective of the paper are good but I'm questioning

(i) the model interpretation and the testing based on
(ii) comparison with measured hydraulic properties and
(iii) numerical experiments using Hydrus 1D.

In short, I propose to use different data sets for model comparison and a more detailed discussion of representing flow processes under dry conditions.

A) In general, none of the discussed models matches the measured unsaturated hydraulic conductivity data (as confirmed by the authors in lines 318-319). The authors hypothesize that these differences between model and measurements are a result of the contrast between measuring soil water retention (and saturated conductivity) in the lab and unsaturated hydraulic conductivity in the field. I agree that conducting measurements in the field will have a big effect and introduce uncertainties - but because the comparison between hydraulic conductivity functions is in the core of this paper, the comparison must be done with measurements that do not have this lab/field-problem. The authors should look for a few measurements from different soil types with very reliable and consistent measurements of both unsaturated conductivity and water retention done in the lab. Specifically, instead of choosing data from UNSODA data base, it would be important to select measurements from papers that are measuring both properties in consistent systems (lab studies).

Reply:
The referee states that the comparison between hydraulic conductivity functions is in the core of this paper, but we intended to focus on the retention curve, as we make clear in the title and the abstract. We recognize that the conductivity curve is important as well, but only devote attention to the effect of the retention curve parameter on the conductivity curve. For a more in-depth treatment of the conductivity curve we refer to Weber et al.

The referee argues we should seek lab data of soil water retention and conductivity measured on a consistent system. The underlying thought appears to be that laboratory data are inherently superior to field data. For applications to practical problems (that by necessity arise in the field) this is not necessarily the case, particularly for conductivity data. Several colleagues with considerable experience in field work have grown rather critical of applying lab-measured conductivities in the field because they often do not perform well. One reason may be that samples that are adequate for the volumetric water content are too small for the hydraulic conductivity: the representative elementary volume for the unsaturated hydraulic conductivity may be larger than the 100 cm^3 often used for soil water retention measurements. Larger samples (1000 cm^3 or more) appear to give more consistent results from anecdotal evidence, but then we do not have the consistent system that the referee prefers.

Based on our fits as well as on earlier reports of conductivity curves based on parameters fitted on soil water retention data, we think that it is better to fit a separate set of conductivity parameters on conductivity data when possible. In this paper, however, we wanted to compare various retention curves. Had we used all three parameterizations with the same conductivity curve, there would have been the risk that the conductivity curve would have had a dominating effect the simulation results. Also, we would not have been able to demonstrate the surprisingly large effect of the choice of the parameterization on the conductivity curve. For this particular goal, our choice was suitable.

We compared the estimated conductivity curves with independent data to present the complete picture to the readership, in order to encourage a critical and sensible use of our new parameterization. If a reader concludes that RIA is a useful full-range retention curve but prefers to independently fit a conductivity curve, we conveyed our message succesfully. This appears to be the case with referee 2. We can try to modify the text to bring this message across more clearly.

B) Related to the problem of inconclusive comparison with experimental unsaturated hydraulic conductivity data is the comparison with numerical simulations between the "VGA" model by Ippisch et al. and the new RIA-model. The results are very sensitive to differences in hydraulic functions at high and intermediate water contents and depend on the accuracy of matching the unsaturated hydraulic conductivity in this water content range. The authors should explain in more detail the differences between the conductivity function of VGA and RIA and – based on comparison with high quality measurements – which approach may be more appropriate.

Reply:
We do not consider the comparison with independently measured conductivities inconclusive. Our message that retention curve parameters do not describe the hydraulic conductivity curve very well came across, but apparently was not perceived as such. The limited transferability of retention parameters to conductivity curves has been known for several decades, so we are not breaking new ground here. We need to try to improve the clarity of our text to communicate this message more clearly.

Independently of this, the shape of the conductivity curve that arises from the RIA parameterization gave quite different and more plausible simulation results than VGA, and we reported this. This comment is related to this particular finding.

Generally speaking, one should fit a separate set of parameters directly to conductivity data when these are available (see above). If one has to rely on retention parameters only, RIA gives a numerically robust set of soil hydraulic property curves, but the simulation results should be applied with care if they are used in practical applications. The referee suggests that we test the ability of the retention parameters to describe the conductivity curve. We hesitate to do so because it has already been established that this does not work very well and we are not challenging this. The referee essentially hypothesizes that retention curve parameters can describe the conductivity curve, but we believe this hypothesis to be false. Such a test would also drift away from the main contribution of the paper, which is to introduce a sigmoidal retention curve without unphysical behavior in the dry and the wet end.

We read our text with the interpretation of the referee in mind. We realized that we unconsciously assumed that the readers shared our views on the limited usefulness of retention parameters for conductivity curves. But for a more optimistic reader like referee 2, our comparison of estimated and measured conductivities is indeed disappointing, and our appreciation of the ability of the estimated curves to sometimes correctly reproduce the shape of the conductivity curve can be a bit bewildering. We thank the referee for bringing this alternative viewpoint to our attention so vividly. We will take into consideration a broader spectrum of opinions on this matter when we rewrite the text in order to avoid unintendingly raising expectations.

The referee mentions the need for high-quality data to perform the test. Much of the data in the UNSODA data base is quite good, and in sheer size and range of soil types, the data base is unparalleled. More importantly, the referee may be too optimistic about the data quality that can be achieved. Unsaturated conductivity data tend to be quite noisy and not always transfer to field conditions well. We distinguish three causes for this:

- the need to measure matric potentials at two heights in the sample that are only centimeters apart. Especially in conductive soils, this leads to substantial errors in the estimates of the matric potential gradient.
- the difficulty with accurately measuring very low fluxes in the dry range. Even when one avoids the need to measure matric potentials below the tensiometer range by imposing matric potentials at opposite sides of the sample, one still has to wait days or more before sufficient leachate is collected to have a valid measurement. If steady state conditions are required this adds days or weeks to the procedure. These long times increase the risk of growth of bacteria or fungi in the sample and the porous plates that are probably needed on the inlet and outlet side of the sample. Furthermore, the small amounts of leachate in combination with the long time intervals make the data collection vulnerable to water losses from diffusion through tube walls or evaporation of the collected leachate from the collection vessel.
- the sample may be too small for measuring hydraulic conductivity. The representative elementary volume may be larger than the sample, and the flow lines in a sample may be forced to be more unidirectional than they are *in situ*.

This poses severe hurdles to carrying out the analysis the referee proposes. Newer setups (such as the HyProp apparatus) produce an unprecedented number of data points (but not in the dry range) at the cost of a relatively small sample size, leading to the size-related problems of the final bullet point.

Given our reservations about using the retention curve parameters to estimate the conductivity curve, we opted for a comparative analysis in the paper and report the main differences between RIA and VGA: the generally faster drop for RIA vs. VGA in the conductivity when the soil becomes slightly unsaturated, and the resulting gradual response of the flux at 2 m depth to rainfall for RIA vs. the rapid and jumpy response of VGA. We are not sure there is an added benefit of a very detailed analysis of a conductivity curve that the referee criticizes below for being insufficiently sophisticated anyway.

We also point out that we present fits to data sets of over 20 soils. In comparison to many of the other papers that introduce parametric expressions of soil water retention curves this is a large number. Only one of these papers included a comparative evaluation of their parameterization by using it in a numerical model, which is the main application of such parameterizations. We therefore already did more work than most to test the performance of our parameterization.

C) *The authors state that the 'behavior' at the dry end with water content dropping to zero for finite pressure values is more appropriate. I agree that at some point even the last molecular layer of adsorbed water will be removed - but can the flow processes under such conditions be described properly with the hydraulic functions proposed in this paper? Are the appropriate physical processes under dry conditions (film flow, vapor transport, ...) described properly with eq. (12) and (13)? As far as I understand, the hydraulic conductivity functions used in RIA (and VGA and VGN) are based on eq. (12) but this expression relies on capillary flow and does not reproduce the physics of film flow (or vapor transport). So, the simulations at the very dry end – that should reproduce the dynamics of water adsorption and film flow – are based on equations valid for capillary flow. The authors should comment on that.*

Reply:
The observation by the referee that the conductivity curve we used is based on capillary flow is correct. We are currently pursuing a way to link improved conductivity curves (based on the papers the referee quotes and other work) to RIA, but we ran into a theoretical issue with the current crop of available curves that has not received attention to our knowledge. We are still working on that. Given the amount of new material (theoretical and mathematical) that we are developing in that project, we concluded that adding it to the work reported here would result in a long, confusing paper with too many lines of thought.

In very dry conditions, vapor flow becomes significant and it can even exceed liquid water flow. When isolated pockets with liquid water and soil air are both present, water moves at least in part by evaporating from one pocket of liquid water and condensing in another, leading to trains of evaporation-condensation sequences. This can only be roughly modeled by a continuum model like Richards' equation through the use of effective parameters and is not represented by any model of strictly liquid flow, be it capillary flow, film flow, corner flow, or a combination of those. The currently available models for film flow and corner flow do not fully capture the architecture of the pore space. They are an improvement over strictly capillary models, but not yet the definite representation of water dynamics in dry porous media. Equations (12) and (13) are definitely less valid for dry conditions than for wet conditions, but more elaborate conductivity models only offer a partial improvement.

The referee requested us to comment on this, so adding a brief discussion below Eq. (13) of the issues outlined above would adequately address this comment. The effect of these processes on the relative magnitude of the fluxes in dry soils may well be very large, but because the fluxes in dry periods are orders of magnitude smaller than those in wet periods, their effect on the soil water balance over longer periods will generally be quite small.

D) Similar to the discussion of the hydraulic properties at the wet end, the authors should compare the model with measurements (also of K(theta)) at very negative pressure levels.

Reply:
This is easier said than done, as can be seen from our discussion above of the limitations on measuring hydraulic conductivities in dry soils. We can measure neither matric potentials below the tensiometer range in soil samples, nor low fluxes at sufficient accuracy. In recent years, sensors that measure matric potentials down to wilting point have become available commercially (https://www.ugt-online.de/en/products/soil-science/tensiometers/full-range-tensiometer/), but they cannot (yet?) be miniaturized to a scale that would make them useful for hydraulic conductivity measurements. We doubt that the data the referee would like us to use will become available in the near future.

There are virtually no water content measurements reported for pF values above 4.2. Measurements in the dry range are limited, and, as Bitelli and Flury showed, often overestimate the water content. We can signal this problem in the paper, but not solve it.

SPECIFIC QUESTIONS
I'm questioning the choice of the title using the terms 'Improved behavior in dry and wet soils' because it was not shown that the 'behavior' was improved.

Reply:
Our parameterization is the only sigmoidal parameterization with a finite slope at saturation and a finite matric potential at zero water content. Both of these are improved behaviors. The mathematical evidence is provided. The referee may have interpreted 'behavior' as 'performance', but the performance, insofar we were able to determine it, improved as well.

Lines 58-62: Please expand this paragraph by 1-2 sentences to explain how the water uptake capacity becomes unlimited.

Reply:
The current paragraph reads:

Fuentes et al. (1991) warned that the asymptotic residual water content at the dry end could lead to a non–converging integral of the retention curve, and showed how this would mathematically lead to a physically impossible unlimited water uptake capacity of a finite soil column. From their analysis follows that this can only be prevented if $n > 2$ in Eq. (1), a condition which is often not satisfied.

We propose to replace it by:

Fuentes et al. (1991) warned that the asymptotic residual water content at the dry end could lead to a non–converging integral of the retention curve when the integration is carried out between the saturated water content and a water content that approximates the residual water content in the limit. In that case, the area below the retention curve becomes infinite. Fuentes et al. (1991) showed that this would lead to an unlimited amount of water stored in a column of a finite length at hydrostatic equilibrium if its height was such that the residual water content was approximated closely at the top of the column. This physically impossible case is only avoided if $n > 2$ in Eq. (1), a condition which is often not satisfied.

Lines 105-117: The authors should expand on the physical differences between adsorption and capillary forces. The entire paragraph is on water retention only and not on water flow under such dry conditions. The authors must discuss different types of flow related to film and corner flow and how this could be implemented (see Tuller and Or, Hydraulic conductivity of variably saturated porous media: Film and corner flow in angular pore space, Water Resources Research, 37, 1257-1276, 2001)

Reply:
The paper focuses on the retention curve, and therefore the paragraph in question dealt with water retention. The conductivity curve is only addressed in terms of the way it is affected by the retention curve parameters in order to explain the significant differences of the simulation results for different parameterizations with nearly identical shapes of the retention curve. We are aware of the limitations of Mualem's (1976) conductivity curve and of the work of Tuller and Or and others on film flow and corner flow but we are still working on that (see above). The reference to Weber et al. points to a method to implement conductivity curves that are not solely based on capillary flow. As explained above, we will add a brief discussion of the issues raised in this and another comment below Eq. (13).

Line 161, eq. (5): I understand that the value of parameter beta is determined using eq. (7). I would have expected that beta should depend on the surface area of the soil (determining the amount of adsorbed water). Could the authors please comment on that?

Reply:
The requirements that the values and the derivatives of two branches of the retention curves match at their junction point were introduced by Rossi and Nimmo (1994). These requirements provide two extra equations that allowed us to solve for two of the variables. The choice of variables for which to solve is arbitrary in principle, but for this particular problem only β and h_d can be expressed in an explicit from that does not require an iterative solution. This strictly mathematical line of argument in no way

negates the point of the referee that β may depend on the surface area of the soil. Equation (7) and the reasoning of the referee are both correct in our view.

All references appear in the discussion paper.

On behalf of all authors,

Gerrit de Rooij