Reply to reviewer # 1 of the revision of ‘Technical note: A sigmoidal soil water retention curve without asymptote that is robust when dry–range data are unreliable’

The comments are in *italics*, the replies in regular font.

L.14: compared to?

Explanation added.

L.45: Please help explain a bit more on why it is impossible so?

This is the Introduction. The peculiar behavior of alpha is the rationale for the theory section of the paper, and it leads to the main objective identified in the following sentence. The nature of the behavior of alpha is discussed at length in the Theory section. I added the elucidation of the behavior of alpha to the objective, to indicate that the paper will deal with this. I refer to my reply top Reviewer 4 in the first round of the discussion.

L.49: when you say nature, i guess you referred to mathematical nature? or physically?

Replaced ‘nature’ by ‘behavior’.

L.51: any citation?

As the sentence states, this finding emerged when I was testing the code and the parameterization.

L. 64: Partition the total water content (potential) into capillary and absorption sections are aligned with the latest breakthrough in defining total soil water potential. Perhaps the authors would like to explain in the introduction a bit the physical consistency between RIA and Ning Lu's latest unitary definition of soil water potential?

Luo, Shengmin, Ning Lu, Chao Zhang, and William Likos. 2022. “Soil Water Potential: A Historical Perspective and Recent Breakthroughs.” Vadose Zone Journal, July. https://doi.org/10.1002/VZJ2.20203.

Luo et al. (2022) is a somewhat provocative paper, and I believe this is deliberate. I do not always fully agree with the theory they propose. I may engage in the debate they initiated in the future, but the discussion requires a rather thorough treatment for which a brief reference is not adequate. The discussion would far extend beyond the scope of this Technical Note, so it is not the best place to start my contribution to the debate.

L 87: please help explain what kind of soil is for this realistic combination of n and alfa values.

L.88: why this value is unrealistic?

I realized I can leave out the segment to which these two comments relate, because the re-analysis of the data of de Rooij et al. (2021) discussed immediately below that is quantitative and rather convincing. This part of the text was therefore deleted. But to answer the question: the SWRC on the semi-log scale is linear for $h < h_j$. Such a long linear stretch is rarely observed.

L. 128: which lower region in Figure 1?

I clarified that the region in which the optimized parameters end up corresponds to the area below the lower bound given in Fig. 3.

L 146: how this could be explained physically? or is it only making sensing in math?

This is strictly mathematical. I am not terribly fond of assigning too much physical meaning to the parameters of SWRC expressions (a view shared by van Genuchten, by the way). That is one reason why the paper threads very lightly on doing so.

L. 153: how could these physical limits be linked to capillary and absorbed water content as assumed in RIA for different soil types?

I do not recommend to do so because of my reservations expressed in the comment above. A soil sample is heterogeneous, and the pore architecture is not very well understood. Different regions in the sample will have different ratios of capillary and adsorbed water (not absorbed!) at a given matric potential, yet we have to describe the end result with only one curve because that is the only thing we can measure.

L. 154: This reviewer assume this is imposed by RIA? and hae is different for different soil types, is there a lookup table for this? And how this lookup table will impact the fitting results and main conclusions?

I do not understand the first question. How can an air-entry value, i.e., the matric potential at which air enters a saturated soil sample for the first time, be smaller than the matric potential at which all water has left the soil sample? The second question seems to miss the fact that RIA has h_{ae} as a fitting parameter, even though that is one of its main improvements over the original equation by van Genuchten (1980). I have never seen tables of air-entry values, although I theoretically computed some myself for different pore radii. (Hydrol. Earth Syst. Sci., 15, 1601–1614, https://doi.org/10.5194/hess-15-1601-2011, 2011).

L. 163: Mathematically?

No, the text is correct.

L. 165: Does it mean this is not anymore closed-form?

Or the correction factor is used to ensure the continuity of RIA and remaining closed-form?

The equation remains closed-form, otherwise the rest of the paper could not have been written. The correction factor shifts the dry branch a little to connect it to the wet branch at the junction point, as explained in the text. The correction factor is a closed-form function of the fitting parameters, thereby ensuring that the RIA remains closed-form itself.

L. 176: Why?

How is this dry branch treated so? (why the wet branch is allowed?) Are there any physical explanation behind, in terms of capillarity and absorption?

The answers are in the text, and in the title. It was already established that continuity of the SWRC at the junction point was no longer guaranteed. Consequently, one of the branches needed to be shifted to restore continuity. If, generally speaking, dry-branch data points are less abundant and less reliable than wet branch data points, why would one shift the wet branch instead of the dry branch?

There is no physical explanation (the reviewer again incorrectly calls the adsorbed absorbed water, by the way). The problem is mathematical, as is the solution. The least reliable of the two branches of the SWRC was shifted by a small distance, often smaller than the thickness of the lines in the plots.

L. 205: Perhaps some considerations behind this multimodality in terms of its physical meaning? for example, when referred to Ning Lu's unitary definition of soil water potential?

Multimodality is usually attributed to characteristics of the pore architecture, for instance when the soil contains of granules that have their own internal pore system but are themselves arranged to form a secondary pore system. It is widely accepted that adsorbed water is dominated by soil texture (because it is located in films), while capillary water is more influenced by soil structure. This implies that, for adsorbed water in particular, the modality of the SWRC will not be affected by the definition of components of the matric potential.

Reply to reviewer #5 of the revision of 'Technical note: A sigmoidal soil water retention curve without asymptote that is robust when dry–range data are unreliable'

The comments are in *italics*, the replies to them in regular font.

GENERAL COMMENTS:
The manuscript presents a method to parametrize the soil water retention curve. The authors build on their previous work, namely Rooij et al. (2021) (https://doi.org/10.5194/hess-25-983-2021), which is further modified in this work to let matric potential at oven-dryness fitted or fixed (log(-hd)= 6.8 cm H2O). The code and a detailed guidance for fitting the presented method is provided in Fortran and available from ZENODO (https://zenodo.org/record/6491979).

This is correct.

The presented fitting method aims to improve the description of the dry end of the soil moisture retention curve with a method that does not increase the number of parameters that have to be fitted, this way could be applied by many users.

If 'fitting method' is replaced by 'parameterization with a modified set of fitting parameters', this is correct.

It would be important to add some information about the Twarakavi et al. (2010) classes under "3.1 Selected soils" paragraph, because it was used for selecting the 21 samples for the analysis.

This is only partially correct. The database was queried for soils with a range of soil water retention points extending into the dry range (pF 3 and up), and with data of the unsaturated soil hydraulic conductivity. About 50 soils were returned. Several of these were discarded for various reasons (small number of data points, data points only covered the first bend of the SWRC, etc.). The remaining set was biased towards sandy textures, so some of the sandy soils were discarded to have a more even distribution over the texture triangle. In the end, 21 soils remained.

That being said, I added an explanation at the start of the Results and Discussion section about the rationale of Twarakavi et al. et al. (2010). The classification they proposed is based on hydrological behavior of their categories, and therefore of considerable relevance for the SWRC. The added paragraph is:

'In the tables that follow, the soil texture classification according to Twarakavi et al. (2010) is provided. The advantage of this classification over the conventional USDA soil texture classification is that it better recognizes differences in hydraulic behavior between its textural classes. This makes it more relevant for soil water flow studies for which the SWRCs are typically used.'

It would be very informative:
- to test the fitting performance on data that has theta-head pairs from the dry range of the soil moisture retention curve,

One of the criteria used when selecting the samples was that they all have dry-range data points, as can be seen in the plots of the SWRCs. As explained in the paper and in de Rooij et al. (2021), these data points are often unreliable though. This was not known to the researchers who made the measurements.

- add descriptive statistics of the 21 samples with information on organic carbon content, sand, silt and clay content, bulk density, pH, calcium carbonate content and information on soil type and summarize based on that which soils were covered in the analysis,

The texture triangle in Madi et al. (2018) gives the sand, silt, and clay contents of the 21 soils. Organic carbon content and bulk density are reported for many samples in UNSODA data base, but the other parameters, including the soil type, requested by the reviewers were not always reported by the contributors to the database. The lowest bulk density of the data set was 1.3 g per cubic cm, because I considered mineral soils preferable. Organic soils tend to have irreversible changes to their soil hydraulic properties when they dry out, making them less suitable for a study with the dry end of the SWRC as one of its focal points.

It is also worthwhile to point out that any soil data other than the data points are of no consequence to the objectives of the paper, and have no effect on the results. I refer to my reply to point 5 of reviewer 2 in the first round of reviews.

- to further analyse why the method is not accurate for clay loam and clay soils and possible further specific soils (e.g.: volcanic soils, salt affected soils, organic soils, etc.), for this many more samples from other soil hydraulic datasets could be used, e.g.: HYPRES and/or EU-HYDI and/or GRIZZLY and/or data from the tropics, etc. or at least mention that this has to be performed in the future.

I am pleased to see that the reviewer sees several avenues for further research emanating from this paper. Pursuing them may be worthwhile, but outside the scope of this technical note. A brief discussion of the poor fits for some of the clayey soils was already added, and I refer to my reply to Reviewer 1 in the first review round. There is not much more I can add to that, nor do I think that is necessary to give the reader a good idea about the strengths and the weaknesses of the SWRC parameterization that is the focus of the paper.

I am reluctant to expand the scope of the paper because that will redirect the focus of the paper away from its main contributions, and lengthen it considerably. I explained my rationale extensively in my reply to point 6 of reviewer 2 in the previous review round. I added the following paragraph at the end of the Discussion:

'This paper focuses on mineral soils with unimodal SWRCs. If an extension to multimodality is desired, Eqs. (12–16) provide a starting point. Further testing on soils with specific characteristics, such as volcanic or organic soils, may be worthwhile. In the case of organic soils, the risk of irreversible changes during drying will require some caution when measuring points on the SWRC.'

The text includes many technical details, some parts could be explained more to ease understanding and use of the method by the readers. It would be important to add a

separate section which:
1. highlights the advantages, disadvantages and limitation of the presented fitting method by comparing its "capabilities" to other existing models to fit the moisture retention curve;

The SCE algorithm is very well documented in the literature. The three references provided give an excellent introduction that allows one to acquire a firm grasp of the intricacies of the algorithm and its operating principle. The user manual gives an explanation that summarizes the algorithm and the way the optimum is iteratively approximated. Comparisons with other algorithms have already been performed for different types of problems and are reported in the cited papers.

2. lists what has to be fulfilled for the proper use of the fitting method – kind of very short practical guidance, e.g.: minimum number of theta-head pairs in the input data required for the fitting, how many theta-head pairs are required between specified matric head values – if that is important, computation of standard deviation of the error in the matric potential, etc.

Please consult the user manual for details on the fitting procedure. Regarding the required number of data points: the location of the data points is rather important, as is an estimate of their accuracy relative to each other. The former was discussed in some detail by de Rooij et al. (2021). The latter is a technical aspect that is covered extensively in the user manual. The same goes for the calculation of the RMSE.

Please find some further comments under SPECIFIC COMMENTS section.
After solving the above mentioned issues the paper can attract wide interest.

SPECIFIC COMMENTS:
L15: why the fitting was performed for only 21 samples? What about the other samples of UNSODA, why were not the other samples used?

See the clarification above.

L16: Please specify what you mean under „The fits are good".

Replaced by: 'The curves fit the data well, ...'

L17: please shortly add why it is problematic/ highlighted: „For some soils, α is very large."

Rephrased as: 'The new SWRC simplifies to an earlier junction model of the SWRC based on a well–known power–law SWRC if α is very large.'

L19-20: would be more informative if the last sentence of the abstract would be a statement which is based on the results, please highlight the main advantage of the method presented in the manuscript, why is it recommended to use instead of other models available from the literature?

The final three sentences of the abstract (in the version seen by the reviewer, the final four) give the three main results of the paper. The main one is that the parameterization fits the data well, but putting that one before the other two does not read so well. With the merging of the final two sentences, it is a little more clear that the final three sentences give the main results.

L82-82: … realistic but large n ($n > \sim 1.4$ and $\alpha > \sim 0.01$) require values …

This sentence was deleted in response to reviewer 1.

L87-88: … For soil 2126 …

There is no difference between the original text and the proposed change (?)

L116-118: please rephrase the sentence starting with „Exploring the parameter space" to ease understanding.

In response to this comment and a comment of the other reviewer, the paragraph was rewritten as:

'Figure 3 shows the band of valid values of h_j enveloped by the limits set by Eqs. (4) and (7). A large part of the parameter space between these limits of h_j has an excessively large $\partial\alpha/\partial h_j$. Finding the optimum will therefore be very difficult for any parameter fitting algorithm. But if the lower limit is not enforced, trial fits showed that the shuffled complex evolution algorithm (SCE, Duan et al., 1992, 1993) consistently ended up in the region of Fig. 1 that lies below the lower limit.'

L137: please add the range in numbers if possible after stating the following: „α can vary over its entire range".

The physical range is any value > 0, which is clear from the equations. But the actual range will be specified by the user on input, so I cannot provide a range here.

L161: … Its value …

I do not understand this comment. Perhaps because the line numbers do not correspond to those in the file I submitted.

L208-210: please shortly add here how these SD were considered during the fitting.

This is described in detail in the User Manual.

L211: please explain why the following was done: „The sample height was set to zero for $h \leq -1000$ cm and for $h = 0$ cm."

Explained in the revised text as:

'The sample height was set to zero for $h \leq -1000$ cm because the variation in the water content can be neglected at low matric potentials. For $h = 0$ cm, it was assumed that the water pressure in the sample was positive everywhere, or that the porosity was measured. In both cases, there is no effect of the matric potential on the local water content, hence the sample height was set to zero to reflect this.'

L228: Please shortly add what the "complexes" mean.

This is explained in the user manual. The references for SCE also explain this.

L252-253: please check if the following is accurate: „The code returns a table of the fitted curve based on the best run". The code might return the fitted parameters or computed theta-head pairs based on the fitted parameter. Is that correct?

The code returns both the fitted parameter values and a table of theta-head pairs based on the fitted parameters. The text is correct.

L262-264: please describe the following sentences to ease understanding: "If these values are equal, the parameter is treated as a fixed value, and the dimensionality of the parameter space is reduced accordingly. The number of complexes is two (for 8 of fewer fitting parameters) or four (see Duan et al. (1994))." E.g.: what do you mean by equal? What does number of complexes mean? Maybe you could provide examples.

The text requires that the reader is somewhat familiar with the SCE algorithm. The introduction to SCE in the User Manual suffices to acquire the required background. For that reason, the text in line 243 indicates that information about the algorithm can be downloaded from de Rooij (2022), so it is not necessary to repeat this in the paper. Providing examples is of little use if one has not read the introduction provided in de Rooij (2022) and unnecessary if one has.

I am not sure what can be unclear about two values being equal.

L344-345: Please add possible reasons for the less accurate fit. Could the fit be improved if the multimodal version of the method is applied for the fitting?

Lines 344-345 do not discuss the quality of fit, but the number of convergence criteria that were satisfied. Depending on how strict or relaxed one sets the convergence criteria it is quite possible to achieve full convergence with dismal fits (criteria too flexible), or have good fits without convergence (criteria too strict). I erred on the safe side and set the criteria rather strict. The User Manual may be of help here.

Perhaps the reviewer refers to another segment of the text, because the line numbers in many comments do not correspond to the line numbers in the text I submitted, for reasons I do not know. But let us assume the reviewer refers to the poor fit for some of the clay soils. As I explain in the text, and as can be seen from the figures, the shape of the RIA function does not describe the shape of the observed SWRC in those cases. That really is all there is to say about it.

Of course, a multimodal model will improve the fit – any fit can be improved by adding more parameters. But because the focus is on data sets with less-than-stellar data in the dry range, increasing the number of parameters would be a poor choice in a data-scarce situation. The risk of overparameterization is too large, in my opinion.

L366-369: the availability of the code with detailed documentation and user manual is plausible, just a minor suggestion: use of the presented method might be easier if it would be implemented later on into Python or R as well.

I do not have the time to do so, but I made an effort in the User Manual and in the comments embedded in the code to describe exactly what each routine does, what it needs on input, what output it generates, and how it communicates with the calling program unit and the modules. Should anybody be interested in converting the Fortran code to another language (that will have longer execution times than Fortran, by the way), this information should be helpful.