Review of Improvement of the soil drainage simulation based on observations from lysimeters (https://doi.org/10.5194/egusphere-2022-274)

The goal of this study is to use a LSM to reproduce soil water mass, volumetric water content and drainage flux observed in seven lysimeters during a period of more than five years. The simulations are performed with three different parametrizations for the soil hydraulic properties, namely the common functions of (i) Brooks and Corey (1966) [BC66], (ii) van Genuchten-Mualem (1980) [VG80], and additionally (iii) a previously proposed "hybrid" approach, where the VG80 retention function is combined with the BC66 conductivity function [VGBC]. Considering standard diagnostic variables, the authors find a best performance with the VGBC approach and a worst performance for the VG80 approach. Ancillary studies further investigated the replacement of heterogeneous, layered soils with uniform properties. The authors note that all the results deteriorate compared to the tests with a heterogeneous profile and conclude that the vertical heterogeneity of the soil hydrodynamic parameters must be taken into account. Finally, the use of PTF-derived hydraulic properties in the simulation is compared to the use of parameters based on in-situ measurements of water content and matrix potential. Basically, the in-situ derived VG80 parameters n differ strongly from the PTF-derived values, leading to significantly different simulation results, which are worse for the PTF-based simulations.

General Comment

Using lysimeter data in soil hydrologic analyses is always exciting because it shows us what we do and do not understand about soil hydrologic processes. And it gives us clues about the reliability or unreliability of local soil moisture sensor readings. So this work is a very good exercise, and the use of lysimeter data for this type of study has merit. Furthermore, the paper is well written and a pleasure to read. However, I have a problem with the main idea of the paper, which is to propose the use of a VGBC parameterization in soil hydrology.

The approach taken by the authors here may be nice from a numerical point of view, but from a physical point of view it must be considered unsuitable. The reason, in short, is that a smooth, continuously derivable soil water retention function (WRC) is combined with an incompatible shaped hydraulic conductivity function (HCC). This does not make physical sense. Furthermore, the comparison of the three functional approaches is most likely biased by problems with the VG80 model when it is used to parameterize the WRC of a fine-grained soil or a soil with a broad pore size distribution (indicated by a parameter value of n close to 1). In such cases, the VG80 hydraulic conductivity curve (HCC) exhibits an abrupt drop near saturation (Durner, 1994). This drop (i) leads to a severe underestimation of the hydraulic conductivity when the prediction of HCC is based on the measured saturated hydraulic conductivity (Vogel et al., 2001) and (ii) negatively affects the performance of the numerical solvers, i.e., their stability and accuracy during the transition between saturated and unsaturated conditions (Ippisch et al., 2006). This could be the reason why the authors of this study limit the smallest value of n to a threshold value (arbitrarily chosen for numerical reasons) of n > 1.09 and also find in the performance comparison that the VG80 model leads to overly wet soil profiles.

To eliminate the well-known artifact of the VG80 conductivity curve for soils with small n three main approaches have been proposed in the past. They are (i) shifting the entire pore-size distribution by an air-entry value (Kosugi, 1994), (ii) introducing an explicit air-entry pressure into the van Genuchten model (Vogel and Cislerova, 1988; Vogel et al., 2001; Ippisch et al., 2006), or (iii) truncating the pore-size distribution (Malama and Kuhlmann, 2015; Iden et al., 2015). Some other workarounds have also been proposed (e.g. Schap and van Genuchten, 2006). The second approach is historically the most commonly used. It effectively eliminates the drop in HCC near saturation and the associated negative effects on the behavior of the numerical solvers of the Richards equation. The drawback, however, is that the resulting WRC is no longer continuously differentiable, i.e., the soil water capacity function becomes discontinuous, which in turn can cause problems with numerical solvers of the Richards equation in some situations.

The VGBC approach adopted by the authors in their study is basically a variant of approach iii, i.e., they leave the RETC in its original smooth form, but limit the conductivity to a constant maximum value reached at an "air entry" value (somehow arbitrarily constructed for soils with small n values).

It is certainly fair to try such an approach. However, the paper fails to convince me that this approach is worth pursuing. An important reason for this opinion is the fact that the results in the paper are not fully comprehensible to the reader, since crucial information about the modeling scenario and especially the hydraulic properties of the soil is missing. So we have to believe the results or not. In addition, the paper has shortcomings, especially in the methods section of soil hydrology (Section 3.1), as will be presented later in this review. As is so often the case in soil hydrology, the devil is in the details, and therefore I recommend reviewing the study again in detail, taking into account the comments below. Specifically, I recommend repeating the analysis (or adding a scenario to the analysis) with modified BC80 HCC functions the remove the abovementioned VG80 artifact. This is probably most straightforward using the HCC functions of Iden et al. (2015, Eq. 18 therein). If desired, I [Wolfgang Durner] would be willing to provide the authors with the respective HCC functions for their lysimeter's retention curves.

SPECIFIC COMMENTS

1. Basic approach:
   As mentioned before, I believe that a mixture of VG RETC and BC HCC is not a good solution to solve the problems with VG80, even though others have tried it and it leads to smooth simulations. The reason is that this is simply unphysical. Above the air entry value, we have significantly increasing water contents, but constant conductivity. This contradicts the soil hydrological evidence.

2. Equations:
   The equations of the model used in the study must be either directly stated or clearly referenced. A statement such as "A complete description of the model equations used to simulate water transport can be found in xxxx (xxxx)" would be appropriate, especially for the soil hydrology processes that are the core of the paper. I have not found this. I understand that the mixed-form Richards equation was used, but with what kind of boundary conditions? This is especially of interest for the lower boundary condition, where Figs. 9, 10 and 12 indicate drainage under apparently unsaturated conditions, which is not possible when the lysimeters are operated with the traditional lysimeter boundary condition (i.e., seepage).

3. Data:
   Which sensors were used? Since in science the reproducibility of results is of utmost importance, the high quality journals nowadays require that all necessary data are given. This bloats the manuscript itself too much, but it is possible to either put the data in data archives or publish them separately in appropriate data journals or attach them directly to articles as additional information. As a specific example, I would actually be interested in repeating the June 2016 G2 lysimeter scenario because the sudden breakthrough of water to the drainage seems difficult to explain with the VG80 data provided. However, with the information currently available, it is not possible to perform such a test and judge the validity of the scientific statements.

4. Results.
   Some of the results are shown as examples, which is fine. However, the reader should have access to the full results. So please use the supplementary material to list data not shown in the manuscript! For me, especially diagrams like figure 1 for lysimeters O1 and G2 are of great interest, also for the five other lysimeters.

5. Lower boundary condition:
   In line 181 authors state "*By assuming the unit-gradient assumption, the drainage at 2 m can be considered equal to the hydraulic conductivity. ksat is then assumed equal to the observed drainage when the soil water content is saturated*" --- The statement is correct if really unit-gradient conditions prevail in the lysimeter. In typical lysimeters, where the water flows freely into the atmosphere, this

would require full saturation of the entire lysimeter(!). In suction controlled lysimeters it is different, but I did not find a statement about this in the paper. Do you have any indication that this assumption can be (approximately) true if the whole lysimeter is not saturated? Or any reference where the validity of this approximation has been shown?

6. Conductivity functions.
   Conductivity functions are key to the outcome of the simulations. As always with simulations, we can say, "What you put in determines what you get out." I would like to see the functions used in this comparison in appropriate graphs. The single Figure 1 is difficult to read and not sufficient. Please see my comments on Figure 1, below. Also, the coefficients of the hydraulic functions used in the simulation study should be listed in a table (perhaps in the supplemental material), as the information in Figure 2 is not sufficient to reproduce the functions.

COMMENTS RELLTED TO SPECIFIC TEXT PASSAGES

1. INTRODUCTION

- line 45. "*Vereecken et al. (2019) suggested a number of directions for improvement: introduce more physical processes such […] improve the representation of […] soil parameters*," --- Agreed. But I do not really see the VGBC approach as an improvement of soil parameterizations in the above-mentioned sense.
- line 56 "*These relationships are simple to parameterize and very stable numerically*." --- There is some irony in the fact that Rien van Genuchten actually developed his parametrization to solve the problem of a discontinuous water capacity function that causes numerical problems in simulations with the Richards equation. So, VG80 should be numerically stable except for cases with very small n.
- line 60 "*However, the VG80 relationships are less stable than BC66 for coarse-textured soil, mainly because of the complexity of the hydraulic conductivity function* (Vogel et al., 2000)." --- In fact, I am not aware of this statement in the Vogel paper. I know VG80 is problematic for coarse grained soils in the dry moisture range, but in that range there is not much difference to BC66.
- line 73 "*We derive their hydrodynamic parameters directly from observation*" --- This is certainly the key to all subsequent results. As already indicated, the documentation on this important point is not sufficiently presented in the paper.

2. EXPERIMENTAL PROTOCOL

- line 85 "*These two sites are separated by a distance of 97 km*." --- Please state here the basic hydro-meteorological parameters: total precipitation (comes too late at the end of the section), total estimated ETp, height above sea level, mean temperature.
- line 101 "*with different layers of limestone more or less cracked*" --- uuh, taking an undisturbed lysimeter in such material is difficult. Described somewhere in literature?
- line 104 "*They are equipped with suction and temperature probes as well as time-domain reflectometry (TDR) probes*" --- please specify the used instruments/sensors.
- line 113 "*The gaps represent up to 15% of the observations for the GISFI site* (Table 2)." --- I tried to figure that out from table 2, but find there a different value, 12%.
- Line 115 "*atmospheric forcing*" – how expressed? How is the upper soil hydraulic boundary condition expressed in the model?
- line 117: "*ISBA model*" --- I would like to see some more equations related to the main hydrological processes in the soil. For example, I have not found the implementation of the boundary conditions, and perhaps the calculation of isothermal vapor conductivity via a function of soil texture could somehow be shown without having to consult Braud et al. (1995).
- line 154. As a soil hydrologist, I am somewhat surprised at this type of notation. Why psi(w) and K(psi), instead of expressing both w and K as a function of psi (which is common, at least in the soil hydrology community)? Of course, this is meant only as a comment and is not of any consequence....

- line 157: "*the more complex closed-form equations from van Genuchten* (1980)" --- No. The equations may look a bit more complicated, but VG's approach is certainly not "more complex". The fact that a simple algebraic equation is very short in one case, while it looks a bit more complicated in the other case, should not be interpreted as "complex" in 2022.
- line 162 "α (m^{-1}) [is] *the inflection point where the slope of the soil-water retention curve (dω/dψ) reaches its maximum value*," --- This is wrong. $1/\alpha$ is inbetween the inflection point and the air-entry value.
- "line 163. "*l [is] the Mualem (1976) dimensionless parameter that determines the shape of the hydraulic conductivity curve*" --- No, *l* does not determine the "shape" of the conductivity curve, but rather the slope of the log K vs. log psi curve in the unsaturated range. The "shape" of the function is unaffected, log K (log psi) remains linear.

3. ESTIMATION OF PARAMETERS

- Line 173 "*The rich data sets collected by the lysimeters allow the derivation of the soil hydrodynamic parameters*"; "*For instance, Fig. 1 plots*" --- Figure 1 is central to the entire paper and its findings. I have a number of comments on it, which are included at the end of my comments here. These data must be given for all lysimeters, as they determine the outcome of the simulations and thus affect all conclusions of the paper.
- line 179: "ω_{sat} *is determined by the 99th percentile of the observed soil volumetric water content*" --- to be sure: this is 6 years * 365 days * 24 values = > 52'000 water content data for each layer? Just make this clear.
- line 178: "*observed ψ-ω relationship at each depth*" --- I assume the depths listed in Table 2? Are the layer boundaries of the different materials in the simulation chosen to be at the mean distance between these observation depths?
- line 182 "*By assuming the unit-gradient assumption, the drainage at 2 m can be considered equal to the hydraulic conductivity*." --- Did you ever observe fully saturated unit gradient conditions in the lysimeter? Saturation just at the base is not a sufficient condition.
- line 193" *Vogel et al. (2000) determined a limit of* $n < 1.3$ *below which Eq.(5) is numerically unstable*." – Well, that's a complex issue. See remarks at the begin of the review.
- line 195. "*The l parameter in Eq. (5) from VG80 is estimated with a simple calibration via ISBA sensitivity experiments with l ranging from -5 to 5*. " --- This is incomprehensible: What exactly was done in this "simple calibration via ISBA sensitivity experiments"? Also, it is suspicious that the optimized values for the GISFI lysimeters are all at the limit of a permissible range. Furthermore, with *l* = -5, we are outside the physically permissible range for many sets of hydraulic functions and might face even increasing conductivity in dry soil (see Peters et al., 2011).
- line 200: "*The derived parameters are presented in Fig. 2*" --- As mentioned above, the parameters (ω_{sat}, ψ_{sat}, α, n, b, *l* and k_{sat}) should be listed (additionally) in a Table, maybe in supplementary material.
- line 215 "*if the volumetric water content presents a slow decrease in summer at a given depth, it is considered that the roots have not yet reached this depth. The root depth is thus fixed at 2 m for lysimeters G3 and O2*" --- Hm, this is really a very large depth for the grass roots. Unusual.
- line 216 "*varies for lysimeters G4, O1 and O3*." --- Would be nice to see this illustrated.
- line 222: "*(not shown*") – Why not shown? In digital format, we do not have space limits in the supplemental information!

4. RESULTS

- line 240 "*we arbitrarily consider that the initial observed and simulated total water masses are equal for the BC66 experiment*" --- ... and how do you get the initial simulated total water mass? Based on what initial conditions in the simulation? And is the initial water content of the VG80 identical to that of the BC66?
- line 249 "*BCVG experiment obtains better scores than the other experiments in more than 42 % of cases*" --- Certainly true, but the differences between the model variants seem to be insignificant. With the exception of lysimeter G4, where the BC66 parameterization leads to a different picture than the others, we can say that the variants give more or less the same results. The fact that in G3 all three

model variants overestimate the water mass might hint on a problem with the initial conditions or the soil mass.

- line 258 "*VG80 obtains weaker statistical scores in 96 % of the cases, because soil water saturation is reached too rapidly*"--- This could be an indication of an incorrect conductivity curve. As mentioned in the introductory section of this study, the use of VG80 is not acceptable for such small values of n, and this result is a strong indication of an incorrect conductivity curve. The study should be supplemented with a modified VG80 conductivity as suggested above.

Table 1

Please add some more key information: USDA soil type (e.g., sandy loam), monolithic or filled, bulk densities.

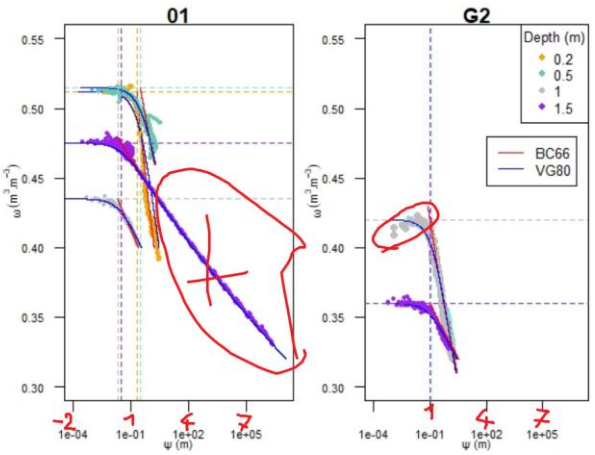
Table 2

Layout is puzzling: two columns for GISFI water content sensors, one column for the respective matric potential sensors.

Table 2. Description of the available observations for each lysimeter: observation period, mean Annual precipitation (Precip) and drainage (Drain). For each type of data, the available depths are indicated (cm). Quality of measurements is given as percentage of missing data: meteo gap for the meteorological forcing, defect for the lysimeters measurements.

Site	GISFI experimental station				OPE experimental station		
Lysimeters	G1	G2	G3	G4	O1	O2	O3
Period	2011-2016	2009-2016		2011-2016	2014-2019		
Precip (mm.year^{-1})	727				876		
Drain (mm.year^{-1})	317	337	115	170	312	304	363
Total Water mass	full column				full column		
Volumetric water content	100-150	50-100-150	50-100-150	50	20-50-100-150		
Matric potential	100-150	50-100-150		50	20-50-100		
Drainage	200				200		
Temperature	50-100-150				20-50-100-150		
Quality of data							
Meteo gap (%)	12				10		
Defect (%)	16	8	23	0	0		

Fig. 1



a) Are these data from five years in-situ measurements (hourly resolution)? Why is there no hysteresis?

b) How are the depicted conductivity data derived? From the paper, I learned that Ksat is derived from a unit-gradient assumption, and relative K-function in the unsaturated range is predicted by the BC66 reps. VG80 model.

c) Why do conductivities decrease with decreasing suction (@1 m, soil G2, grey dots)

d) How are the RETC data for O1 @1.5 m derived? Such experimental data cannot be obtained this far into the unsaturated range! Moreover, a water content of 35% is impossible at a suction of 1E+5 m. Note that this suction condition I beyond oven dryness, i.e., ω = 0!
e) What's the meaning of the dotted lines (I assume psi_s and ω_s, but name it in the legend or caption!)
f) Why do we find such strongly different slopes of RETC in a packed lysimeter (G2) with homogeneous)!) soil? What are the bulk densities?
g) Where are the data for O2, and O3, and for G1, G3 and G4? → supplemental material.

Fig. 2

a) Ksat – I am not able to decipher the unit. 10^6 m/s ???
b) The *n* values are very low, close to 1, but in this figure it is impossible to distinguish values near one. Please list the values also in a table.

Fig. 9

a) Why do we observe outflow in a system that does not reach saturation at the bottom? Are these suction lysimeters?

TYPOS AND MINOR ISSUES

- Terminology. For me it is puzzling to speak of "experiments" when actually different simulations are meant. The "experiment" to me is the physical experiment where a system is manipulated to observe a response. Perhaps "model variants" or "model approaches" is more appropriate?
- line 83: This is an international journal with many readers not familiar with french terrestrial research units: please define GISFI and OPE upon first occurrence.
- line 95: which bulk density?
- line 200: Typo "lystimeters".
- line 203: replace "deep" by "depth".
- line 243 „*average biases of 18.1 kg (19.18 and 21 for BC66 and VG80)*" --- Keep an eye on your digits: Better "18.1 kg (19.2 kg and 21.0 kg for BC66 and VG80"
- line 277 "if" ??????????
- line 304 "dynammic"

Literature cited

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