

Numerical study of the evaporation process and parameter estimation analysis of an evaporation experiment

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We would like to thank the reviewers for their valuable suggestions to improve our manuscript and we revised it according to their suggestions as listed in detail below.

Reply to reviewers' comments (reviewers' comments are italic)

Editor:

I was wondering about the sentence "... a soil-atmosphere boundary layer dominated regime (regime I) in the saturated region ..." in the abstract. The meaning appears not clear. I think this can be clarified later.

We have reformulated the sentence to make it clearer.

Reviewer #1: N. Shokri

General Comments

... however there is still need to explain the physical aspects of the problem in more detail and especially discuss more about the potential impacts of the coupling between the external boundary conditions and the internal transport properties of porous media on the evaporation rate. Some of the assumptions are too simplified and the authors at least should discuss the possible consequences of these simplified assumptions (see comments below).

We clarified the physical model and its assumptions, according to the reviewers suggestions.

Specific Comments

Page 7386, line 11: It is helpful to mention some words about what you mean from the “drying front” (is it the interface between unsaturated and dry zone?). Some people define the drying front as the interface between the saturated and unsaturated zone, so it might be confusing for the readers...

We changed the text to define “drying front” more precisely by: “... a drying front (interface between unsaturated and dry zone with very steep gradients) forms ...”

Page 7390: In your analysis, where is the contribution of the convective transport of water vapor above the soil surface in supplying the total flux? To me, it seems you just considered the vapor diffusion from the surface through the overlying viscous boundary layer (VBL), while considering Figure 1 in your manuscript, there is air flow above soil surface which for sure induce vapor convection. Therefore, neglecting the convective part is not physically correct. The reason that you don't see the effects of this assumption in your analysis probably is in the end you fit r_b on the obtained results. I am not saying you have to consider the most complicated case, but saying you have to be aware of the simplified description you have provided and have to inform the readers and explain this in the manuscript.

Since the air in the evaporation chamber is turbulently mixed, the water (chemical) potential is uniform throughout the chamber. As the air velocity in the chamber is not high we do expect a viscous boundary layer at the soil surface. As diffusion is the dominant vapour transport process inside the soil, we use the (homogeneous) potential inside the chamber as upper boundary condition. We used the same model to fit an experiment conducted in the setup studied in this paper and obtained excellent agreement between modelled and measured data [Schneider *et al.*, 2006]. We added a sentence to the description of the simulated experiment to make this clearer in the paper.

Insert in experiment description: The air inside the chamber is turbulently mixed to ensure a uniform potential throughout the headspace.

Page 7390: In equation (5), you have assumed a constant value for r_b which is indeed a very simplified assumption. In fact the thickness of boundary layer is zero at the entrance of the soil surface and increases by increasing the distance

from the leading edge. When I read the manuscript for the first time, I expected more theoretical development/improvement in addressing the coupling between the external boundary condition with the internal transport of porous media in supplying the evaporative demand. There are too many fitting parameters in equation 5 (the fitting parameters related to ψ and r_b). . . . where is the effect of evolution of water content at surface and its coupling with external VBL in modification of mass transfer coefficient at the surface?

We think that there was a misunderstanding of our boundary layer concept. In our approach, the boundary layer *only* accounts for the soil-atmosphere boundary at the top of the sample and denotes the diffusive interface which is caused by the fact that turbulent eddies of the atmosphere in the head space cannot penetrate the surface. Thus, when approaching the surface from above, eddies become successively smaller and in a very small band directly at the surface, diffusion is the dominant process. In contrast, the vapour diffusion which takes place when the drying front moves into the soil is automatically accounted for by the Richards' model since it also simulates vapour diffusion inside the soil. In fact, during regime II r_b becomes practically irrelevant since the major resistance is caused by the diffusion of water vapour through the dry zone. We described the model and our conceptual approach in more detail to clarify matters.

Again this approach is supported by the good agreement between experiment and simulation in *Schneider et al.* [2006].

Page 7394, line 18-19: Change "only" to "mainly" or "mostly". In addition, I would add something like "relatively" or "rather" before "a constant value of", because the evaporation rate during stage 1 is not completely constant, but "relatively" constant due to the evolution of liquid curvature at the evaporation surface affecting the capillary pressure gradients and consequently the upward liquid flux.

We agree that in regime I, the outflux is only nearly constant due to the evolution of liquid curvature and the corresponding pressure gradients. The model accounts for changing pressure gradients and corresponding upward liquid flux. Indeed the flux is slightly decreasing. However this effect is so small (6th or 5th significant digit) that we had called it "constant". We clarified this in the text.

Page 7395, line 10-13: There are several studies showing that at the end of stage 1 evaporation, liquid continuity and hydraulic connection between receding drying front and evaporating surface is interrupted resulting in formation of a dry surface layer limiting total evaporative flux from porous media. Recently I wrote a paper (Shokri et al. (2009), Water Resour. Res., 45, W10433, doi:10.1029/2009WR007769) which I believe has direct relation with the current manuscript (it is always awkward to point out a lack of reference to your own work, but I do believe it is very related to the argument provided in this section of the paper). It was shown experimentally that at the end of stage 1 evaporation, receding of the liquid meniscus from the evaporation surface is resulted in formation of a dry surface layer and marks the onset of stage 2 evaporation. In other words, during stage 2 evaporation, liquid is transported upward via capillary induced liquid flow to the bottom of the dry surface

layer, vaporize at that level and then vapor diffuses through the dry layer to enter the atmosphere. This observation/analysis clearly explained the transition from stage 1 to stage 2 of evaporation. In the current manuscript, I think it is better to explain the physically based reason of the abrupt transition rather than arguing based on the drop in the “effective” hydraulic conductivity. I have the same concern about page 7395, line 27-28.

We agree that interrupting liquid connectivity and the resulting formation of a dry surface layer occur at the transition to stage II. However, we do not agree that they are the reason for transition to stage II evaporation. As our model calculations show, already during stage I water is transported by capillary induced liquid flow to the surface (and it is easy to verify this from experimental data by calculating the amount of water evaporated during stage I). The drying of the surface layer is the consequence of the fact that the capillary induced flow is no longer sufficient to sustain the evaporation rate. This results in a drying of the soil surface.

Page 7396, line 3-4: Explain the reason of “the drier the sample, the less important is the resistance of the boundary layer”

In our definition, the resistance of the boundary layer only applies to the atmospheric boundary layer, not to the dry zone in the soil. If the soil is dryer, an increasing distance in the soil has to be covered by vapour diffusion. Thus the effective resistance inside the soil becomes higher than the resistance of the actual boundary layer at the soil surface.

Figure 4(b): In profile (2), why water content is reduced almost uniformly through the entire sample? I expect existence of an interface between saturated and unsaturated zone after 35 hrs of drying, while in your simulation, you have obtained almost a spatially uniform water loss from the entire column. In the beginning of the process, one can expect intuitively that air molecules invade the porous medium from top surface while bottom of the sample remains saturated, thus there should be an interface between the saturated and partially saturated zone close to the surface.

1. Of course drying occurs always at the top first and the water content of lower regions can only decrease if a continuous gas phase connection to the soil surface exists. However, as the gas phase occupies the largest pores such a significant gas phase conductivity can already exist at very small air saturations.

2. While in sands the pore size distribution is rather uniform leading to very low unsaturated conductivities in the dry range and sharp infiltration and drying fronts, the situation is different in materials with a rather wide pore size distribution like loams. There, unsaturated conductivities remain high up to quite low potentials. Thus the soil is capable to sustain the stage I evaporation rate for a longer time resulting in a more uniform drying of the whole soil sample. This is the case for profile (2). We added an expanded explanation in the text.

Figure (8): Changing the atmospheric condition at $t=62$ (hrs) influenced the outflux computed by the assumption of no vapor transport (blue curve), but why the jump in the atmospheric condition at $t=196$ (hrs) does not have any influence on outflux (blue curve)?

Without vapour transport enabled, the conductivity in the dry soil is practically zero and the change in conductivity when the potential is made even lower is negligible. We already explained this in the text. We added a sentence “For more explanations see section 3.2.1” to the figure.

Technical corrections

General comment: Use thicker lines in all figures. The lines are too thin ...
We adjusted the line size for all figures

Equation (2): Define θ_r and θ_s .
We defined both symbols in the text.

Equation (4): Show the derivation of equation (4) or at least give a reference. It took a while for me to understand the equation... Equation (5): I would first introduce the Kelvin equation and then present equation (5). Not all readers are familiar with these equations...
We added a more detailed description of the model to the paper.

Equation (6): Introduce the parameters and give reference to Levenberg-Marquardt algorithm!
We inserted a reference and explained the parameters of the Levenberg-Marquardt algorithm.

Page 7386, line 14: change “By using the boundary condition changes” to “By changing the boundary conditions”.
We changed the formulation accordingly.

*Page 7394, line 20: “measurand”?!
We changed “measurand” to “measured quantity”.*

*Page 7409, Table 2: I think you mean p^w and not p_w .
We corrected p_w to p^w .*

Reviewer #2

Specific Comments

p. 7393, l.7-9: For my first reading, it was hard to understand this sentence. Please make it clearer corresponding with the relative value of parameters shown in Fig.12-14 (also for the subscript "0"). "parameter i" should be "parameter j" according to Eq.(7).

We have reformulated the text to make the sentence clearer.

p. 7395, l.23-: Why don't you mention about the general interpretation of relative sensitivity coefficient? Not everyone is familiar with it. Is there any meaning for positive or negative value? Larger absolute value means higher sensitivity. And the meaning of "zero crossing" is not clear.

The sensitivity coefficients s_{ij} are a measure how much the quantity i changes when changing parameter j . When s_{ij} is positive, quantity i increases when increasing parameter j , when it is negative, quantity i decreases. The larger the absolute value of s_{ij} , the more changes quantity i for a given parameter change. When encountering a zero crossing of s_{ij} , quantity i changes in opposite directions before and after the crossing, while it is not affected by parameter changes directly at the zero point. We added this to the text.

p. 7402, l.7-: Same as relative sensitivity coefficients, not everyone is familiar with response surface, general interpretation is needed. Which shape is good for inverse fitting and how is correlation between two parameters.

We now explain the concept in more detail in the materials and methods section 2.3.

Technical Comments

1. p7389, Eq.(2): Define θ , θ_s , and θ_r . τ is equal to 0.5? It's not used as a fitting parameter in following of this article.

We have inserted the definition of θ , θ_r and θ_s into the text (cf. also reviewer #1). The value of τ was indeed set to 0.5, we have added a list of inverted and fixed parameters where we describe the numerical inversion.

2. p7389, Eqs.(3) and (4): Define K_l , g , z , and t . Use the same variable for liquid water content, θ_l or θ . 3. p7390, Eq.(6): Define variables.

We added the missing definitions to the text. We now only use θ_l for the liquid water content

4. p7390, l.18-24: Show the reference of this inverse procedure.

The name "Monte-Carlo Levenberg-Marquardt" was introduced in this paper to describe the combination of randomly chosen initial values with a Levenberg-Marquardt iterative parameter optimisation. A reference to the Levenberg-Marquardt algorithm itself was added to the text (cf. reviewer #1).

5. p7391, l.9: *Give the length of soil column and initial condition.*
We included the initial condition and the sample height into the text.

6. p7391, l.17: *matrix potential → matric potential. Can be found in several sentences.*
We substituted matrix potential by matric potential in the whole text.

7. p7391, l.22-24, l.1: *Give the equation converting permittivity to water content.*
In the optimisation procedure we did not convert permittivity to water content, but we calculated permittivity from the water content. We added the equation used.

8. p7392, Eq.(7) middle term: $(t, z, p_j) \rightarrow m_i(t, z, p_j)$
we changed the middle term to $\left. \frac{\partial m_i}{\partial p_j} \right|_{t, z, p_j}$ to make clear that the derivative of m_i in respect to p_j , taken at position (t, z, p_j) is meant.

9. p7393, l.5: *You have to make clear which parameters to be fitted before here.*
We have included the information in section 2.2.

10. p7395, l.16: *saturated hydraulic resistance → hydraulic resistance (reciprocal of hydraulic conductivity) It is not only for saturated case.*
In the mentioned sentence we compare the saturated resistance = reciprocal of the saturated conductivity, which is the lowest possible resistance, with the resistance of the boundary layer. If the lowest possible resistance is still higher than the resistance of the boundary layer, regime I does not exist. We made that clearer in the text.

11. p7395, l.17: *Give the actual value of K_s . Is it 0.005cm/h?*
We inserted the actual value of K_s into the text.

12. p7396, l.12: *“shape of the soil water capacity curve” → “shape of the soil water retention curve”. Is there any special reason to use “water capacity curve”?*
We replaced the term soil “soil water capacity curve” by “soil water retention curve”.

13. p7398, l.15: *Fig.8 seems to be showing for the three steps boundary condition. Are you mentioning about the 1st step at 70 hr? It makes readers confuse.*
It is correct that we refer to the first step at $t = 70$ h. We made that clearer in the text.

14. p7401, l.1: *Define Δh .*
We added the definition of Δh to the text.

15. p7402, l.14: *Since relative values are used for axes, you should mention $n/n_0 = 1$.*
We have added this to the text.

16. Table 2: $p_w \rightarrow p^w$
17. Figure 3: $p_w \rightarrow p^w$
We made the first correction, but could, unfortunately, not find p_w in Fig. 3.

18. *Figure 5 Legend: “high” alpha*

We corrected the legend

19. *Figure 6 middle: Although you’re explaining about the regime I, it is hard to see. Upsize this reason.*

We added a figure with the detail plot of potential sensitivity from $t=0$ to $t=100$.

20. *Units are needed for all variables.*

We added units to all variables in the paper.

21. *Use the same term for j^w . “Water flux at the upper boundary”, “outflux”, or “evaporation flux”*

We now use the term “evaporation flux” throughout the paper.

Reviewer #3: H. Fujimaki

General Comments

This work investigated the effect of multi-step atmospheric boundary condition on reliability of determined hydraulic functions including dry range in which traditional evaporation methods using tensiometers cannot cover. This topic would be informative for many readers of HESSD and manuscript is generally well written. However, there are several points to be corrected or clarified before acceptance for publication. As the authors admit, the experimental setup causes drop in soil temperature in the initial stage. Latent heat loss must be compensated by horizontal and upward conduction from the column walls. I would recommend to improve the experimental setup such that automatically-controlled radiation keeps the soil temperature the same as ambient one.

The current paper is not about optimisation of a real experiment, but about the study of a virtual one to get an idea of important processes and the identifiability of hydraulic parameters. However, the reviewer shows with his statement a way how a real experiment could be forced to behave more like the idealised one we simulate.

The authors also admit that the multistep procedure forces the investigator to consider hysteresis for accurate determination of hydraulic properties. I suppose that the effect of hysteresis is not critical in low pressure head range. However, the authors should evaluate the validity of neglecting hysteresis. A simple hysteresis model such as Scott et al. (1983) may be valid and the authors are able to do it.

We stated in the paper that “any change in the direction of flow leads to hysteresis, which was not considered in the simulation. Further work is needed to investigate if the influence of hysteresis can be seen in simulations and experimentally and how severe it changes the system.” This probably was too strong a statement. Actually we are quite sure that the effect of hysteresis in this kind of experiment is rather small. Hysteresis is most pronounced in coarse textured porous media and in the wet range of experiments. In our numerical multi-step experiments, the switch occurs only in the dry range where water vapour is the only relevant transport mechanism. We changed the discussion in the text to make that clear.

I think that additional retention data using vapor equilibrium or psychrometer are required to precisely determine retention curve in dry range. Deviation from “true” retention function may be avoided if such information is provided.

The use of additional data is always helpful in obtaining a better characterisation of the porous medium. We studied in the paper already the effect of adding an instrument which measures potential with an infinite range precisely. However, to our knowledge such instruments still do not exist for in situ measurements in a soil sample.

Specific Comments

P7389L5: Realistic hydraulic functions should be used in numerical experiments. In my knowledge, van Genuchten’s hydraulic functions are not suitable for describ-

ing hydraulic functions in low pressure (dry) range. I have never seen a soil that can be appropriately fitted with van Genuchten's retention curve in whole saturation range. The authors should consider to use Fayer's or similar hydraulic functions proposed to cover dry range. (Fayer, M.H. and Simmons, C.S. (1995) : Modified soil water retention functions for all matric suctions. Water Resour. Res.,31: 1233-1328)

The question of the applicability of certain hydraulic parametrisations in the dry range is intensely discussed and there have been several proposals to improve this. In the experiments we conducted [Schneider et al., 2006] we could get a nearly perfect fit also in the very dry range using just an ordinary Brooks-Corey model. As the Brooks-Corey model is perfectly equivalent to the van Genuchten model in the dry range, we do not see any need to use a different parametrisation.

P7391L12: Table 1 and Fig.16. Again, realistic hydraulic functions should be used. I have never seen a sandy loam whose saturation becomes zero at -100 kPa or silt whose saturation becomes zero at -1 MPa. The authors should use parameter values that have measured including dry range.

We agree with the reviewer that the low saturations at low potentials look confusing. In fine textured soils there is a certain quantity of water which cannot be removed by simple desaturation or even drying at room temperature. This is considered in the van Genuchten parametrisation by the parameter θ_r . As it is impossible to estimate both θ_s and θ_r by an evaporation experiment alone, we set θ_r to zero for all experiments and just fitted θ_s , which then corresponds to a kind of "available water content". This explains also the rather low values of θ_s for sandy loam and silt. We added a short explanation to the text to clarify this. Notice that this is true for all kinds of Multistep-Outflow experiments as well.

P7391L21: Table 3. Accuracy in the measurement of J_w should be given in absolute value (mm/h), not in relative one (%), because it depends on accuracy in the measurement of air humidity or weight of the core. In Fig.15, standard deviation of J_w seems to be around 0.01 mm/h with an interval of about 1h. I think it is unrealistic to assume such a high accuracy. Usually, it is difficult to measure sharp drop or increase in evaporation rate as shown in Fig.8 and 15.

Accuracies were determined experimentally with an error analysis by Schneider et al. [2006] and these values were used for the simulations. The novel evaporation measurement uses infrared absorption spectroscopy for vapour concentration measurements which is very accurate and also allows the measurement of sharp drops or increases.

P7400L16: Regime does not back to Regime I. In Regime I, evaporation rate must be constant under a constant meteorological condition and soil temperature. In Fig.15, no such stage is found in (b) and (c). In (a), the second constant evaporation rate was formed before entering Regime II.

Figure 15 is actually a rather bad figure for identifying the regime changes as it shows the measured data, which has some noise added, and the worst accepted and the best rejected fits. The question here is: is it reasonable to accept the worst accepted and to

dismiss the best rejected fit. We think this question can be answered with yes for all three plots. The regime change is also hard to see, as such a long time span has to be plotted in one picture. For the sand in Fig. 15, we agree that the switch occurs before regime II is reached, this is also stated in the text (p. 7399, ll. 1ff). However, in the sensitivity analysis on p. 7400, we only refer to the silt.

Figure 15: Why initial evaporation rate could not be reproduced for the rejected ones? Usually, r_b can be determined from the initial evaporation rate and thus should not be treated as a fitting parameter.

Due to the highly nonlinear nature of the soil hydraulic parameter functions, any gradient based parameter estimation scheme can get caught in local minima. This occurred in some of the rejected schemes. We agree with the reviewer that it would probably be a good thing for this virtual experiment to first estimate r_b by fitting only the stage I evaporation. However, this is not realistic for a real world experiment, as the influence of surface temperature changes is too high in this stage. Standard evaporation experiments do not control the surface temperature, therefore they need to fit r_b together with the other parameters.

Technical Comments

P7387L17: At this line, ψ_m has not been defined.

We changed the text accordingly.

P7387L21: Generally, "matric potential" is used to refer pressure in soil water. Please consider to replace "matrix potential" to "matric potential".

We changed the text accordingly.

P7388L9: measurand \rightarrow measurement?

We changed "measurand" to "measured quantity"

P7389L9: theta is not defined.

We added the definition.

P7390L10: "of atmosphere" should be added after "partial pressure of water vapour".

We changed the text accordingly

P7392L20: Please consider to add "value" after "jth parameter".

We changed the text accordingly

P7395L16 Definition of "saturated hydraulic resistance" is unclear.

We have added the definition of "saturated hydraulic resistance" to the text.

P7401L2: At which depth does the changes in the sign of delta-h occur? What is h?

We added the definition of Δh to the text. The change of Δh occurs "in close proximity to the evaporating surface", according to the plots in the original publication it depends

on the parameter and is within the upper two centimetres of the soil.

Figure 16: Scale of potential should be unified among the three figures.

We agree that typically it is more convenient to have unified scales in the figures. However, in that specific case the potential scales were adjusted to optimally visualise the curves. A common potential scale would make it much harder to see the important features.

References

Schneider, K., O. Ippisch, and K. Roth, Novel evaporation experiment to determine soil hydraulic properties, *Hydrol. Earth Syst. Sci.*, 10, 817–827, 2006.