

Interactive comment on “Field scale effective hydraulic parameterisation obtained from TDR time series and inverse modelling” by U. Wollschläger et al.

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Reply to the comments of Sacha Iden

We thank Sascha Iden for his comments on various issues of inversion procedures. While we agree that improvements on the technicalities of inversion methods are possible, and essential for some problems, we do not think that this will significantly deepen our understanding of the processes and of possibilities of their simplified representation for a case as described in this paper.

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1) The presented study is not innovative from a methodological point of view. Neither is it technically fully state-of-the-art because it neglects recent trends in nonlinear optimization methodology and does not address the issue of uncertainties of model predictions.

We trust that this comment refers exclusively to the inversion method employed and fully agree. We regularly use various tools, e.g., numerical solvers for differential equations, without improving their methodology even in cases where there is a general need for improvement. The focus of this paper is on estimating parameters for a highly simplified model of a complicated set of processes and with this respect, we believe that the paper does have its merits. For some comments concerning the application of global optimisation methods please refer to issue 8) raised by G. de Rooij and issues 1) and 2) by Th. Wöhling.

2) It does not become clear to me what the authors mean when they refer to 'effective soil hydraulic properties' or 'parameters'. [...]

Concerning the terminology or 'effective hydraulic properties' please refer to our reply to item 1a) of A. Coppola. With respect to the upscaling problem the aim of our study was to estimate the hydraulic parameters of our soil profile directly at the scale of interest which basically was done in order to circumvent the upscaling problem. Concerning the issue of upscaling of the estimated hydraulic properties to the field scale we will add a paragraph to the discussion of overall results in a revised manuscript of the article. Here please also refer to our response to issue 3) raised by G. de Rooij.

3) The uncertainties of the estimated soil hydraulic properties (retention and conductivity function) are not quantified [...]

We agree with the reviewer, but would like to point to the full issue. Uncertainties of our problem may be referred to three hierarchical levels: (i) values of the parameter

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estimates, (ii) shape of the functions for the respective material properties, here $\theta(h)$ and $K(\theta)$, as is mentioned by the reviewer, and, most importantly, (iii) observed and deduced phenomena. We did address (i) in the traditional way and (iii) through an admittedly small set of inversion runs. This suffices in our view.

4) Is it really possible to predict correctly the soil water fluxes if both the soil hydraulic properties and the upper boundary condition are simultaneously adjusted during optimization? [...]

A major message of this paper is that, within the parametrisation chosen, adjusting the hydraulic properties alone cannot reproduce the observed time series $\theta(t)$ but that the introduction of the crop factor leads to a qualitative improvement.

5) How do measurement errors in the upper boundary condition propagate into inaccuracies of the estimated hydraulic properties? [...]

We believe that measurement errors of the upper boundary condition are rather small since the meteo variables are measured accurately and on-site. The *modelling error*, i.e., the translation of the meteo variables into the water flux through the boundary, is thought to be significant, however. This actually is a major message of the paper, as has been pointed out before.

Concerning the reviewer's suggestion to run numerical simulations before, we completely agree in principle but point out the following: (i) Done in earnest, this would be a very significant effort since a high-dimensional space, much higher than the 17 dimensions we used for the inversion, would have to be explored. As a starter, various parametrisations of the soil hydraulic properties would have to be studied, including parameter-free formulations, and the impact of a temporal variation of the vegetation cover would have to be explored. Multi-dimensional and multi-scale heterogeneity would have to be added and a number of processes that are obviously missing in our simplified model would have to be accounted for. (ii) Obtaining an optimal field-scale

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effective model for soil water movement under highly variable forcing is a challenge that will stand for some time to come. This paper can only be a small contribution towards this goal.

6) Why aren't parameterizations other than van Genuchten-Mualem tested and their performance compared in terms of model adequacy. [...]

We agree that deploying different parametrisations would give additional freedom. Choosing MvG is a model decision. Indeed, it is one among many others some of which would have significantly deeper impact, e.g., adding a dynamic vegetation model.

7) The manuscript fails to mention a recent trend in soil hydrology which consists of making use of high performance global optimization techniques to overcome the difficulties of classic, gradient-based optimization algorithms. [...]

We agree with the reviewer that global optimisation is a current trend. One will have to see what is coming out of it eventually, after the heuristic methods have been put on solid footing and after their value for identifying simplified models of complicated realities has been assessed. We will mention global optimisation algorithms in a revised version of the manuscript. Please also see our reply to issue 8) raised by G. de Rooij.

8) Unfortunately, the manuscript does not show figures of the soil hydraulic properties at all [...]

We will add a figure in a revised version of the manuscript.

9) The number of references (44) is too large. [...]

References fulfill two functions: (i) referring the reader to work that has scrutinised

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a given statement and (ii) giving credit to the producers of preceding work. We re-checked our list and found it to be alright.

10) P 1490 L 2-3: *I think it is the heterogeneity of soils that necessitates the concept of effective properties. [...]*

Please refer to issue 1a) raised by A. Coppola.

11) P 1490 L 3-5: *It is stated that small scale laboratory experiments do not yield hydraulic parameters which can be transferred to the field scale. [...]*

There are no laboratory measurements available for the soil at our site. A comparison of the different methods and discussion of the related problems was subject of many previous studies (please refer to the respective citations in the introduction) and is not the objective of this article. Our intention was rather to directly measure at the scale of interest and to avoid the well-known issues of parameter transfer from the laboratory to the field.

12) P 1490 L 13-15: *Apart from the processes not included in the applied model, the incorrect parameterization of the soil hydraulic properties is an additional source of error [...]*

Please refer to item 6) above.

13) P 1490 L 20: *the inclusion of preferential flow at this point appears speculative to me, because this matter has not been analyzed by this study.*

We will remove "like preferential flow" from the abstract but leave it in the discussion section of the paper. Please also refer to issue 11) raised by G. de Rooij.

14) P 1490 L 23-25: *As far as I understand the term effective properties, they imply*

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that the soil or part of it (e.g. a layer) is treated as uniform, as well.
Agree.

15) P 1491 L 2-9: *The cited experimental methods to be evaluated by inverse modeling are all laboratory methods. [...] How does this solve the problem you refer to?*

It is stated that *direct* methods using small samples yielded inaccurate results and that the accuracy was improved by developing inverse methods on laboratory samples. In the following paragraph we address the problem of transferring these data to the field scale and summarise the limited number of studies which aimed at the inverse estimation of hydraulic properties from field measurements, meaning directly at the scale of interest. This, in our opinion, is a straight forward way towards the problem we refer to.

16) P 1491 L11-12: *Please note that the inverse methods cited have the major advantage that they are less time-consuming than traditional, static or steady-state experiments.*

We completely agree with the reviewer but compared to transient field measurements like the one we conduct in our study they are much more labour intensive and expensive. We will clarify this point in a revised version of the paper.

17) P 1491 L28-30: *If the soil is heterogeneous (and this is what you emphasize in the manuscript), is it still true that single sensors at each depth can yield representative information on the major status variables of soil water flow?*

The major heterogeneity in a layered soil occurs between the layers, not within. Please also refer to our reply to issue 3) raised by G. de Rooij.

18) P 1493 L 99: *do you mean 'quasi steady-state'?*

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Here, we indeed mean 'quasi-linear': 'quasi steady-state' would imply quasi-linearity, but quasi-linearity, meaning the dynamics can be linearised, is a larger class of states.

19) P 1494 L19-20 *The TDR probes were calibrated in water and air but they were not calibrated against soil water contents. [...]*

It is not clear to us what the remark of the reviewer exactly refers to but the accuracy of a TDR measurement is indeed on the order of about $\pm 2 \text{ m}^3 \text{ m}^{-3}$ what is – to our knowledge – in the range of most methods measuring volumetric water content.

20) P 1496 L 5: *α is closely related to the inverse of the air-entry value only for relatively large values of n .*

Changed - please see reply to item 4) raised by G. de Rooij.

21) P 1496 L19-22: *Wouldn't the use of scaling factors for the van Genuchten Mualem parameters improve the model because the increase in clay content is continuous? [...]*

In our opinion, i) this type of heterogeneity is only useful in multidimensional models and ii) introduces a large number of additional parameters.

22) P 1497 L 1-2: *Can such a material (gravel with loamy matrix) be adequately described by the van Genuchten Mualem parameterization of the soil hydraulic properties?*

If the material is well mixed and we can assume an REV we do not see a reason why not.

23) P 1497 L14-16: *Setting parameter θ_s to the porosity is a source of error [...]*

Please refer to our reply to issue 1c) raised by A. Coppola.

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24) P 1498 L 6-7: *Wouldn't it be more efficient in terms of computing time to restrict the profile depths in the simulations to 2 m and impose a free drainage boundary condition at the lower boundary? [...]*

Please refer to the reply to item 4) raised by Th. Wöhling.

25) P 1500 L 18-20: *Does the inclusion of θ_s in the optimizations necessarily lead to problems that suffer from nonuniqueness? [...]*

This statement indeed is somewhat unfortunate. Please see response to issue 1c) of our reply to the review of A. Coppola. We will rephrase this sentence in a revised manuscript.

26) P 1500 L 20-21: *More recent studies by Schaap et al. imply that a value of -1 for the Mualem connectivity parameter seems to be a better choice. Why do you stick to 0.5? [...]*

The reviewer is right that the connectivity parameter could also have been included in the inversion procedure. We deemed it as a factor of lesser importance, however, and dropped it for the sake of a simple model.

27) P 1502 L 17-18: *Two different rooting depths are compared, 8 and 12 cm. If this reflects the range observed during the soil excavation, you should maybe indicate this in order to justify explicitly your approach.*

We will rephrase the sentence to "Since our information on rooting depth is based on a simple visual inspection during the soil profile excavation, the influence of rooting depth on the modelled water content evolution was investigated by repeating the simulation using a rooting depth of 0.12 m."

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28) P 1502/1503 L 25-28 / 1-3: *Did you obtain identical parameter estimates or at least identical soil hydraulic properties or was it just the temporal dynamics of the water content that was 'similar' [...]*

Since the deviations between measured and simulated water contents were unacceptable, we directly searched for a process which could be responsible for the deviations and did not analyse the inverted parameters which supposedly are not meaningful anyway.

29) P 1503 L 5-6: *This statement is entirely speculative because it relies on the assumption that the only error source for the simulation results are the boundary conditions! [...]*

We agree with the reviewer that there are many error sources which of course will affect the perfect reproduction of the measured water contents. However, as explained in more detail in our reply to issue 2a) of A. Coppola), the FAO Penman-Monteith reference (not potential) evapotranspiration requires scaling if the specific crop differs from the reference crop. Hence, from a scientific point of view our approach appears justified.

30) P 1503 L 19-21: *Note that this means to optimize simultaneously the soil hydraulic properties and the upper boundary condition! To me this appears to be a rather risky adventure. Note that the estimated values for κ are around 0.6 in all cases (Table 3), which means that the overall potential evapotranspiration is reduced by 40%. This has a huge influence on the mass balance.*

Please refer to our comment on item 1) raised by G. de Rooij and 2a) by A. Coppola.

31) P 1503 L 22-23: *'were again conducted using four different rooting depths' ? the studies so far have used two different rooting depths. [...]*

Please refer to our response to issue 5) raised by Th. Wöhling.

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32) P 1504 L 3-7 P 1504 L 14-16: *If your optimizations suffer from these problems, why do you report your results without running a better optimization algorithm? [...]*

Please refer to issue 8) raised by G. de Rooij.

33) P 1504 L 24-25: *ok, but the cumulative water flow leaving the root zone varies dramatically, between 3 and 11 cm! [...]*

The cumulative flow leaving the root zone calculated from the simulations with $RMSE < 0.013$ lies within a range between (119 and 138 mm) which is very narrow and it definitely does not vary dramatically even if we start the simulations with two different initial parameter sets. We will indicate that we refer to the simulations with $RMSE < 0.013$ here. Concerning the estimation of groundwater recharge we will mention the uncertainty of the boundary conditions in the revised manuscript.

34) P 1506 L 23-25: *Why should the soil hydraulic properties change with time? What are potential processes occurring at this site causing them to vary? Please be more precise. In its current form, this statement appears rather isolated and speculative.*

Before the test site was installed it was used for agricultural purposes and the uppermost horizon was ploughed regularly. Since the beginning of the scientific experiments the site was planted with grass and the soil surface was not reworked any further. Hence, we expect a structural transition at least of the plough horizon occurring over time. Furthermore, the soil is cracking due to dry periods in summer. We expect these and further processes to change the hydraulic properties of the test site over time. We will mention this in the revised manuscript.

35) Page 1507 L 5-7: *This is only partly what you have done. [...]*

We will extend this sentence to "The inverse estimation of hydraulic properties in

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combination with a crop factor which scales the FAO Penman-Monteith reference evapotranspiration, ...”

36) Page 1507 L 8: the wide range of hydraulic states covered by the data occurs in the topsoil but not in deeper layers (see the measurements in Figure 2). [...]

Agree, but this is probably also the range of naturally occurring states. We will mention this in a revised version of the article.

37) Page 1507 L 13-15: I agree, but will we ever be able to get these data with the required accuracy? And what will soil hydrologists do if this is not possible?

Obviously, we cannot look into the future. However, there already exist trustworthy methods for measuring water fluxes in the atmospheric boundary layer, e.g., eddy covariance, and we do not perceive fundamental obstacles for accurate measurements of the water fluxes across the soil-atmosphere interface.

38) Legend is missing in Figure 2

We will move the legend for the TDR measurements further downwards in the figure.

39) It is not mentioned which value was used as minimum allowed pressure head at the soil surface during the Hydrus-1D simulations

The absolute value of the minimum allowed pressure head at the soil surface was set to 150 m. It will be added in a revised version of the manuscript.

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