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Hydrology and Earth System Sciences Discussions

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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General comments

The authors present results of a study on inverse estimation of soil hydraulic properties from transient water content data measured at different depths in a field soil. Inverse estimation methods are nowadays routinely applied in soil hydrology. Therefore, 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. Some points require particular attention during the revision of the manuscript.

It does not become clear to me what the authors mean when they refer to 'effective soil hydraulic properties' or 'parameters'. I think it is the heterogeneity of soils that necessitates the concept of effective properties. It appears therefore favorable to include a paragraph on the two principal methods of upscaling in soil hydrology: forward and inverse upscaling (see for instance: Vereecken et al., 2007). This could be inserted easily at page 1491, line 24 before concluding that inverse upscaling is a 'pragmatic path to follow'.

The only uncertainties quantified by the authors are those of the estimated model parameters. The uncertainties of the estimated soil hydraulic properties (retention and conductivity function) are not quantified, although this can be achieved easily by means of the first-order-second-moment method. See Durner et al., 2008, for a brief technical description and examples for layered soils and weighable lysimeters. The significance of this in the context of the presented study is that the authors estimate both soil hydraulic properties and the upper boundary condition (through the reduction factor κ) simultaneously by inverse modeling. I suspect that this increases the uncertainty of the soil hydraulic properties and this should be clearly demonstrated in a quantitative manner in the article.

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? I think this should be confirmed by a study using synthetic data before real data are analyzed.

How do measurement errors in the upper boundary condition propagate into inaccuracies of the estimated hydraulic properties? Since bottom fluxes cannot be measured in the field and the upper boundary condition is subject to considerable measurement error, the mass balance of soil water remains unknown. I wonder whether the correct determination of soil hydraulic properties is possible at all under such conditions. I think this should be confirmed by a study using synthetic data before real data are analyzed.

Why aren't parameterizations other than van Genuchten-Mualem tested and their performance compared in terms of model adequacy. There are different metrics for comparing model performance, like AIC, BIC, KIC (see the recent review of Yeh et al., 2008). I think the exclusive treatment of one single model of the hydraulic properties is a major shortcoming of the manuscript. A problem with the van Genuchten-Mualem parameterization is that θ_s is set equal to the porosity of the soil which is physically questionable and furthermore restricts the possible shape of the van Genuchten retention function. This problem is neither addressed by the authors. The same holds for Mualem's connectivity parameter l which is neither included in the optimization nor do the authors assess its influence on the simulation results by a sensitivity analysis. Without testing alternative models of the soil hydraulic properties, the conclusion drawn by the authors that errors in the upper boundary condition are the only cause for the observed mismatch between simulations and measurements is wrong.

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. A few words on this subject would improve the article. Whether these methods can be applied in all studies on vadose zone water flow (the comment by T. Woehling appears to point in this direction) must be questioned, because global optimization techniques based on evolutionary algorithms often require too many function evaluations (evolution is a very slow process).

Unfortunately, the manuscript does not show figures of the soil hydraulic properties at all, it exclusively reports values of the estimated model parameters. In recommend to add these figures because they are much more straightforward to understand and therefore can be used for comparing the results of different estimation strategies tested in the study.

The number of references (44) is too large. Since this is not a review article, I suggest to reduce the number and cite only those publications which are directly related to this work.

Specific comments

P 1490 L 2-3: I think it is the heterogeneity of soils that necessitates the concept of effective properties. This heterogeneity does, however, not necessarily lead to difficulties in the determination of effective properties. In fact, strongly heterogeneous soils may not have effective properties at all (see Durner et al. 2008 for an extensive study on lysimeters containing layered soils).

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. How about the site and soil dealt with in this study? How do the inversely estimated hydraulic properties relate to those determined on small samples, if there are any?

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 which is not mentioned in the abstract.

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.

P 1490 L 23-25: As far as I understand the term effective properties, they imply that the soil or part of it (e.g. a layer) is treated as uniform, as well.

P 1491 L 2-9: The cited experimental methods to be evaluated by inverse modeling are all laboratory methods. Why do you state that 'It turned out [...] that these methods yield rather inaccurate results. This led to the development ...', if the methods mentioned thereafter relate exclusively to laboratory studies as well. How does this solve the problem you refer to?

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

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

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information on the major status variables of soil water flow?

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

P 1494 L19-20 The TDR probes were calibrated in water and air but they were not calibrated against soil water contents. From my experience, I conclude that the water content measurements can be $\pm$ 2

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

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? As Hydrus-1D supports this feature, one could make use easily of this concept.

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?

P 1497 L14-16: Setting parameter θ_s to the porosity is a source of error, because it is impossible to fully saturate a soil in the vadose zone in a field situation. The maximum relative saturation which can be achieved is probably in the range of 0.8 to 0.9. The problem with the approach is that fixing this values reduces the flexibility of the van Genuchten retention function which may contribute to the mismatch between simulations and observations discussed later. As a consequence, I suggest to treat θ_s as a free parameter during optimization and check whether this leads to better results. In order to keep the number of degrees-of-freedom low, you could alternatively fix parameter θ_r to reasonable values (maybe zero) because the measured water contents are never below 0.1, i.e. the soil does not become dry enough to support the unique estimation of θ_r.

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? Such a boundary condition is often used in situations where the groundwater table is far below the surface. Making the profile shorter would decrease the number of nodes of the FE mesh by a factor of two leading to much quicker numerical solutions. Since the inverse problem requires repeated numerical solutions of the Richards equation, the authors would gain resources for further studies like those suggested above. The approach selected by the authors is physically alright, but it appears numerically inefficient.

P 1500 L 18-20: Does the inclusion of θ_s in the optimizations necessarily lead to problems that suffer from nonuniqueness? Is this statement based on a rigorous tests using your dataset or is it based solely on speculation?

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? Does a change of the parameter affect the results? Did you check this by a sensitivity analysis?

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.

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' ('very similar', 'almost identical', 'identical'?). This is an important point because it indicates whether the soil hydraulic parameters can be identified uniquely given the boundary conditions and data included in the objective function.

P 1503 L 4: This is probably all that you can do given that no replicates are available for the rainfall measurements. But it is regrettable that replicates are not available because rainfall measurements are error-prone.

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! This means to neglect entirely all other error sources in the model simulations, namely errors in the soil hydraulic properties, errors in the Richards equation, and errors caused by representing a heterogeneous soil as an array of layers assumed to be homogeneous or at least assumed to be amenable to a homogeneous treatment in the model. In the following, the authors focus on a correction of the upper boundary condition by introducing a correction factor for the potential evapotranspiration. Given the above shortcomings, this means to base the following analysis on an improper scientific reasoning.

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.

P 1503 L 22-23: 'were again conducted using four different rooting depths' – the studies so far have used two different rooting depths. This means that we now vary soil hydraulic properties, upper boundary conditions and the rooting depths as well. Indeed, one may argue whether one should treat the rooting depth as additional degree-of-freedom in the optimization (see the comment by T. Woehling).

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? Do you finally trust your results or don't you?

P 1504 L 24-25: ok, but the cumulative water flow leaving the root zone varies dramatically, between 3 and 11 cm! How does this compare to your conclusion on page 1506, line 22-23: 'could be applied for estimating groundwater recharge'

P 1506 L 18-21: I don't share the authors' view that the fluxes are correct and can be reliably predicted. This statement must be based on a thorough uncertainty analysis which is not carried out in this study.

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.

Page 1507 L 5-7: This is only partly what you have done. The best results were obtained by fitting hydraulic parameters and the upper boundary condition simultaneously and that it different from what you state here.

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). Therefore, the reliability of the parameter estimates should be much lower in deeper regions of the soil than in the topsoil.

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?

Technical details

Legend is missing in Figure 2

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

References

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