Hydrol. Earth Syst. Sci. Discuss., 11, C5277–C5290, 2014
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Hydrology and Earth System Sciences
Discussions

Interactive comment on "Estimating flow and transport parameters in the unsaturated zone with pore water stable isotopes" *by* M. Sprenger et al.

M. Sprenger et al.

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We thank Christine Stumpp for her very thorough and constructive review of the manuscript. She points out several possible improvements that we are thankful to work on before handing in the revised manuscript. In the following, we will give a short answer to each of the points of Christine Stumpp.

Comment: Please emphasize that you only get information about transport (dispersivity) by using isotopes; it cannot be estimated from water content or suction data
Reply: The fact that transport parameters are not possible to derive from hydrometric data is a strong argument to include pore water stable isotope data and we will emphasize this point more strongly.

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Comment: Why are you using deuterium contents only? What about oxygen-18? Wouldn't it add to get information about parameter uncertainty?
Reply: We have analyzed the pore water for both deuterium and oxygen-18, but we only include deuterium in the inverse modeling approaches, because the applied soil physical model (HYDRUS) cannot account for fractionation processes due to evaporation. In addition, the measured 18O and 2H contents are highly correlated (according to the local meteoric water line). Hence, the gain of information is limited by including oxygen-18 and the uncertainty would not be reduced. In contrast, the relative errors of the stable isotope analysis were slightly smaller for deuterium, since it is less affected by fractionation processes than 18O and due to the higher precision of our measurements.

Comment: At the three sites, the number and time point of isotope depth data are different, which has to be discussed. Having more data in the objective function (e.g. for Hartheim) most likely improves the parameter identification. Further, the model efficiency can be different for summer or winter if incorrect assumptions regarding snow melt or transpiration were made.
Reply: We will emphasize in the discussion more thoroughly the differences of the available data and a possible influence on the parameter identification. We will discuss differences in efficiencies between summer and winter and will include a discussion of the possible errors due to false assumptions made upon transpiration and snow. (In a future modeling setup we are planning to include a time variable leaf area index to account for the temporal dynamics of this control on transpiration.)

Comment: The functional evaluation procedure calculating transit times and giving annual water balance certainly adds to the interpretation of the results. With some exceptions, the annual water balance calculations are quite similar. Are they significantly different? What is the uncertainty range? The authors did a sensitivity analysis for the parameter identification. Can this be further used in the forward calculations to give ranges of the calculated water balance components?

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Reply: We will apply statistical tests to see if there is a significant difference between the different water balance calculations. We will use the best 10 percent of the inverse derived parameter sets to run the model in forward mode, calculate the water balance components of each run and include ranges in the components in Figure 5. We believe such an approach will also help to see the uncertainty of the transit time calculations. Therefore, we will also add parameter uncertainty ranges to the cumulative breakthrough curves in Figure 6.

Comment: I was expecting a more thorough discussion about the gained soil hydraulic parameters using the different approaches. Are there any data available, e.g. measured saturated hydraulic conductivity or porosities, to compare the results?
Reply: We will try to get more data regarding measured soil hydraulic properties (such as saturated hydraulic conductivity or porosities) to include them in our discussion. However, we believe that information gained from laboratory measurements at soil cores or via field measurements are only of limited value comparing to parameters derived from inverse model approaches due to the different spatial scales. As we have pointed out in the introduction of our manuscript, we try to estimate the parameters on the scale of interest and the transferability of the parameters across scales (soil core to soil profile) is critical.

Comment: Care needs to be taken with the interpretation of dispersivities at some sites and with some approaches (see specific comments). A "spin-up" period of two years is not enough for sites with mean transit times > 2 years and therefore dispersivities in larger depths cannot be estimated.
Reply: Only the study site in Hartheim has a "spin-up" period <2 years. We will test if a longer spin up period will change the result and use the time series of Hartheim in sequence to double the simulation period. For Roodt and Eichstetten, we will analyze if a shorter spin up period will have an influence on the simulation.

Comment: Abstract ln 16-18: it sounds like the authors did some additional HYDRUS modifications; as an existing modified version was used, it is more appropriate to write

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"and a modified version of HYDRUS was used allowing deuterium loss during evaporation". By the way, HYDRUS should be written with capital letter throughout the manuscript.
Reply: We will change this part as suggested for clarification.

Comment: 11204/11205, ln 24/ln 1, 6: "satisfying model performance", "satisfying model efficiencies": these terms are rather unspecific and subjective; re-phrase to be more specific (applies to entire manuscript)
Reply: We will change these terms like "satisfying model performance", "satisfying model efficiencies" in a more specific way by referring to the efficiency criteria (Kling-Gupta-Efficiency)

Comment: 11207, ln 8-13: referring to stream flow studies in catchments is not required
Reply: We have included such references upon request from the editor before publication was possible in HESSD.

Comment: 11208, ln 3/4: "so far not been": better to write "rarely" or rewrite the sentence stating that it has not been tested how isotope depth profiles can improve the inverse modeling procedure. We previously used isotope depth profiles at four locations in Ghana to calculate groundwater recharge rates; among other methods, we also used the isotope data in HYDRUS 1D to identify flow and transport parameters (Adomako et al. 2010, HSJ, 55, 1405-1416).
Reply: We are aware of the study presented by Adomako et al. (2010). However, they do not specify how the parameters have been estimated. "The soil hydraulic parameters were determined assuming gravimetric equilibrium of the water contents with depth during the observation in June/July 2008 (Table 1). The measured water contents and isotopes were used to fit Ks and αL. However, these values should only be considered as an order of magnitude, because little information about the profiles was available" Adomako et al. (2010). Thus, we did not refer to that study. Nevertheless, we will include the study as an example, where pore water isotope data was included

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in the parameterization of a soil physical model.

Comment: 11208, ln 12: “long time spans”: there is a limit of time spans though; the expression is rather subjective and should be re-written to not cause misunderstanding. Dispersion causes mixing and therefore, the seasonal signal gets attenuated and after a certain time cannot be used to track water particles anymore.
Reply: We will substitute “long time spans” by “months to years”. The time span is generally dependent on the depth of the isotope profile.

Comment: 11208, ln 18, 21: “soil hydraulic properties” rather than “soil physical” (applies to entire manuscript)
Reply: We will change this as suggested for the entire manuscript.

Comment: 11208 ln 20-23: terms like “adequate”, “most reliable” are not specific; I reckon the authors want to achieve high accuracy between simulated and measured data and later see whether the identified parameters make sense for the tested soils
Reply: We are referring to the goal of getting a “well-calibrated” model as described by Gupta et al. (2005, Encyclopedia of Hydrological Sciences, Chapter 142), which is later discussed in the section 4.1. Therefore we will rephrase it as follows: “. . .result in a “well calibrated” (Gupta et al., 2005) parameter representation?” and “. . .to estimate the solute transport parameters afterwards most reliable?” by “. . .to estimate the solute transport parameters afterwards the best way to derive a “well-calibrated” soil physical model?”

Comment: 11209, ln 21: despite the information given in Table1, more information about soil water measurements is required in the text: what sensors? how many? how close to profiles? - 11210, ln 26: how was precipitation collected?
Reply: The sensors (5TE sensors) are specified in the Table 1. We will include the information that at the site Roodt, at each depth 3 sensors have been installed within a distance of 3 m from each other and an average of these 3 was calculated for each depth. The isotope profiles were taken within 3 m distance to the soil moisture sensors.

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For Eichstetten, seven soil moisture sensors were installed; each representing one depth. The biweekly samples of precipitation were taken as bulk samples and at the study site in Roodt, additional event based (every 4 mm) samples were taken, and paraffin oil was used to prevent evaporation fractionation.

Comment: 11211, ln 1: I reckon the authors analysed the water and not its vapour using the equilibrium method; be more specific here
Reply: We will change for clarification as follows: "The rainwater isotope analyses were also done with the Wavelength-Scanned Cavity Ring Down Spectrometer (Picarro, Santa Clara, USA), which was coupled to a vaporizer to analyze liquid samples."

Comment: 11211, ln 1-4: "minimize the influence of initial conditions" sounds awkward; to also consider the initial deuterium concentration, the time series were extended; more information is needed about these other sampling locations close by: which locations? how far were data extended? it could influence your model accuracy at the different locations
Reply: We will rephrase the sentence as suggested and we will include more information about the other sampling locations (GNIP stations for Roodt and meteorolical station Schauinsland for Eichstetten).

Comment: 11211, ln 6: Water flow instead of water transport
Reply: We will change this as suggested.

Comment: 11212, ln 8: Why did the authors choose a LAI of 2 for the grassland sites? It seems rather low but certainly is justified if only little vegetation was present.
Reply: Since no LAI measurements were done at the studied grassland sites, we had to apply values from the literature which are given by Breuer et. al (Ecological Modelling 169 (2003) 237–293; 10.1016/S0304-3800(03)00274-6).

Comment: 11212, ln 26: I reckon the delta values + an arbitrary value were used for conversion into positive numbers because you cannot calculate with "negative" concentration data. Either this information has to be added or the sentence deleted as it

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could be misleading
Reply: It is correct that we added an arbitrary value to the delta values and we will add this information here.

Comment: 11213, ln 3: add "(data not shown)"; it would be even more important if the d2H/d18O values are similar to the individual Local Meteoric Water Line
Reply: We will add "(data not shown)" and refer the ïĄď2H-ïĄď18O relation to the LMWL of Trier for Roodt, and the LMWL of Weil for Hartheim and Eichstetten, which have been published by Stumpp et al. 2014; Journal of Hydrology (doi: 10.1016/j.jhydrol.2014.05.034)

Comment: 11213, ln 5-9: generally, this statement is correct. If choosing the example of Maloszewski et al. (2006) it is worth mentioning that this was even for sediments without vegetation. Probably referring to one of the previously mentioned lysimeter studies containing soils and not sediments and having vegetation instead of being bare, would be even more appropriate and comparable to your sites here.
Reply: We will refer here to the study by Stumpp et al. 2012, Vadose Zone Journal (doi: 10.2136/vzj2011.0075), who studied the percolation in lysimeter with natural soils and vegetation cover and did not see any isotopic fractionation due to evaporation in the lysimeter outflow.

Comment: 11213, ln 20: "were" instead of have been
Reply: We will change that as suggested.

Comment: 11213, ln 24: "according to the soil description": I am wondering about the choice of soil horizons at the Roodt site. it was mentioned earlier that the B horizon ends in 50 cm bgs followed by a weathered C horizon. Why not combining horizons A and B, having also similar textures, and getting a second set of flow and transport parameters for the C horizon.
Reply: The Soil moisture time series for 30 and 50 cm depth are more similar to each other than compared to the soil moisture in 10 cm. Therefore, we decided to include the

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soil horizon between the A and the B horizon, rather than distinguishing between the B and C horizon. We also believe that it is crucial to get the water flow in the upper part of the soil as correct as possible, in order to keep the errors in the actual soil evaporation and root water uptake (root zone upper 20 cm) small. In addition, there was no soil moisture data for the C horizon, which would bring problems in the parameterization of the soil hydraulic parameters, because they would then depend solely on the isotope profile data. In order to keep the number of parameters for the three study sites the same, we do not want to include a third horizon. However, we see the limitations and will consider the third horizon in a follow up study on the Cambisol in Roodt.

Comment: 11214, ln 1: a spin-up period of two years is probably not enough for the Eichstetten site when looking at the transit times (Figure 6). Here, transit times are larger than two years which needs to be discussed. It is apparently also not enough for Hartheim regarding the IPA and 2SA calculations because the deuterium content below a certain depth equals the initial average (Figure 2). Therefore, the yielded dispersivities should be taken with care and do not reflect actual dispersivities! Please add these points to the discussion
Reply: The spin-up period was >5 years, >4.5 years and 22month for Roodt, Eichstetten, and Hartheim, respectively. We will include this information directly. For Hartheim, the time series of isotope data in the precipitation is short and we will include this limitation leading to biased dispersivity values in the lower soil horizon in our discussion.

Comment: 11214, ln 14, Table 2: how were these initial parameter chosen? Were the initial parameters gained from PTFs in these ranges too?
Reply: The initial parameter range was decided in a way to allow the SCE algorithm to search for a parameter set in a rather wide parameter space, since it is a global search algorithm. Thus, the initial boundaries will have only a limited influence on the final (optimized) parameter set.

Comment: 11215, ln 11: "(PTF)" has to be introduced here and not in ln 2, 11216
Reply: We will change that as suggested.

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Comment: 11215, ln 15-17: was an initial range for dispersivities chosen too?
Reply: The initial range of the dispersivity was the same for the IPA as for the other inverse model approaches. We will include this information here.

Comment: 11216, ln1, 5-6: if the dispersivity was optimized, this procedure can be considered as an inverse procedure too. I was wondering why the authors have used the forward simulation procedure at all; two more sentences could be added here (e.g. PTFs most simple approach if only texture data are available); additionally, the results of the model performance are only briefly mentioned in the text later. Instead of preparing additional figures, it would still be worth giving the model efficiencies in Table 3.
Reply: We will rephrase the sentence to clarify that the approach that used PTFs to derive soil hydraulic parameters and inverse modeling to estimate the dispersivity parameter. We will include the KGE of the simulations run with the parameters derived from PTFs in Table 3.

Comment: 11216, ln 23-28: this functional evaluation procedure is really good to see whether differences in inversely determined parameter really lead to differences in flow and transport; 2-3 sentences on its relevance should be added here to make it easier for the reader to follow why water balance and transit time were calculated. It could also be added to the objectives of the entire study
Reply: We will add more information on the relevance of the water balance and transit time calculations here and in the introduction.

Comment: 11216, ln 28: why intermediate and how were these two events chosen? arbitrarily? please be more specific
Reply: We chose intermediate rain events, because such events are on the one hand big enough to generate water percolation in deeper depth (and not being fully evapotranspired) and on the other hand such rain events are more representative than heavier rain events, which are less likely to occur. The timing was chosen to show the pronounced differences of the processes over time, due to seasonal variation in the evapotranspiration and its consequences for the root water uptake and evaporation. In

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addition, influences like antecedent moisture and rain masses following the traced rain event are major drivers for the transit times. We will add such information about the conditions, how they will be different in spring and fall, and how they might influence the calculations.

Comment: 11217, ln 22: this information (soil moisture sensors) needs to be given in the methods section
Reply: We will add the information about the uncertainty ranges in the methods section.

Comment: 11220, ln 6-7: Not the high Ks but rather the very low saturated water content causes the high seepage water fluxes in first place. The low saturated water content results in low effective water contents (resulting also in the short transit times, Figure 6). Hence, water more quickly reaches deeper soil regions and is evaporated or taken up by plants anymore.
Reply: We will include the role of the low saturated water content value of the unconstrained isotope profile approach (uIPA) for the water balance and the transit time.

Comment: 11220, ln 24-25: see previous comment
Reply: We will include the role of the low saturated water content value of the uIPA for the water balance and the transit time.

Comment: 11221, ln 9-10: it is difficult to judge the results in terms of actual processes at the study sites as no independent measurements were done; therefore, the interpretation should be limited to the comparison between modelling approaches.
Reply: Simulations that would not be "in line with understanding of the processes" would need to be discarded. However, we will include a comparison between the modeling approaches.

Comment: 11221 ln 26-28 (and following section): it has been shown that the accuracy of ROSETTA is limited if textural classes are given only (Vereecken et al. 2010) which needs some discussion. Furthermore, I don't understand your statement why

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an accurate application of PTFs requires homogeneous flow. As you correctly mention later in the manuscript, the Richards equation assumes homogeneous flow in soils and therefore, it is no explanation if a PTF works in one place and not in the other place.
Reply: We will include the limitation of the PTFs when considering only textural information in our discussion. The statement regarding the homogenous flow was aimed to show the advantage of inverse modeling approaches to get parameters that result in a better representation of the processes since these methods will fit the parameters in a way that the water flow is well simulated. As such, the parameters will be effective parameters that hold information about non-homogenous flows, which cannot be represented in the model, but might be compensated by the parameter set. We will change this section accordingly for clarification.

Comment: 11222, ln 7-8: be more specific; in all approaches inverse modelling was used, but additionally having information about soil water content improved the modelling efficiency which is actually expected.
Reply: We will discuss more pronounced the differences between the approaches that did not use any inverse modeling, but pedotransfer functions to derive the soil hydrological parameters, and the MOA and 2SA, to show the opportunities that come with a site specific parameterization compared to a parameter set derived from data bases.

Comment: 11222 ln 14: "reasonably well"; are there any data available for comparison and to be more specific here?
Reply: We will add the following for clarification: "...reasonably well in terms of soil moisture dynamics and isotope composition of the pore waters."

Comment: 11222 and 11223: see earlier comment about dispersivites at Hartheim and Eichstetten
Reply: We will include the above mentioned limitations for Hartheim. As stated above, the spin-up time for Eichstetten of over 4.5 years will be enough for minimizing the effect of the initial deuterium concentration in the soil profile.

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Comment: 11223, ln 2-3: I would not say it is at the lower end compared to the dispersivities found in the lysimeter studies. Here, dispersivities in the soil layers were 3.9-4.7 cm (Stumpp et al. 2012) and 6.8-8.1 cm (Stumpp et al. 2009a) which is in the same order of magnitude to your results.
Reply: We agree and will change accordingly this section to "...are in the same order of magnitude of the data presented in the review..."

Comment: 11223, ln 6-7: certainly, isotope depth profiles are beneficial. However, it also requires isotope data in precipitation over long time spans which has to be available; this points should be added to the discussion and later considered in the conclusions too
Reply: It is correct that isotope data of the precipitation is crucial and this will be added here and in the conclusion.

Comment: 11223, ln 8-19: It was difficult reading this section and following your thoughts.
Reply: We will rephrase this part in order to make sure that our point that isotope profiles are beneficial to derive site specific information about the water flow and the accompanied dispersion processes.

Comment: 11225, section of transit times: I was missing some discussion on the water balance calculations here too. Does the functional evaluation now show that results are all similar anyway - no matter of soil hydraulic properties when also considering the uncertainties? Or are there crucial differences in flow and transport?
Reply: We will include in this section the above mentioned uncertainty estimates for the water balance and transit time calculation to show if there are actually significant differences between the different approaches. We focus in our discussion on the transit time estimations, because these kinds of calculations would not be possible without estimating the dispersivity parameter with the knowledge about the pore water stable isotope data. Thus, the transit time estimations are a new feature which should be emphasized with this section. However, the water balance calculations will be included

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in the revised manuscript.

Comment: Table 1: soil moisture data, Hartheim: check the spelling of "-30"; the second horizon in Roodt ends in 50cm and therefore it is not >25 cm; do you have any information about C(v) horizons at the other sites?
Reply: The spelling will be corrected. As already stated above, the first horizon at Roodt, the A-horizon, ends in 25 cm depth and so does the first layer in the set up of the model. On the decision how to subdivide the soil profile into layers, we refer to the reply above.

Comment: Table 1: please add the maximum root depth in the table
Reply: We will add the maximum root depth.

Comment: Figure 1: please change the range of the y-axis for Hartheim (e.g. 0-0.6) to better see differences/similarities between observed and simulated values; additionally, it is difficult to see some of the overlapping simulated soil moisture curves (e.g. 30 and 50 cm in Roodt, uIPA)
Reply: We will adjust the y-axis accordingly. We will change the curves (e.g. by dashed lines) to make the differentiation between the different simulated soil moisture time series easier.

Comment: Figure 2: uIPA Hartheim: what is the reason for the oscillations in the deeper part of the profile? Is it possible that these are numerical oscillations?
Reply: We will test if a smaller space between the nodes in the profile will help to overcome possible numerical oscillations

Comment: Figure 3: please indicate in the title what white and dark green means; the darker the more narrow is the parameter range - did I get it right?
Reply: We will indicate in the figure caption that the darker the green, the narrower the parameter range.

Comment: Figure 5 and 6: please indicate in the title that it refers to seepage water

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fluxes and transit times in 200cm depth
Reply: We will indicate in the title that the seepage fluxes and transit time calculations refer to 200 cm depth for Roodt and Eichstetten and to 120 cm for Hartheim

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