

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

C. Stumpp (Referee)

christine.stumpp@helmholtz-muenchen.de

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The manuscript presents a study testing three different inverse modelling strategies to estimate soil hydraulic properties and dispersivities. All of them include the use of vertical soil water stable isotope profiles. The big advantage of using stable water isotopes next to soil moisture data is that additional information about solute transport and time scales (transit times) is gained. The results of study show that highest model efficiencies were achieved when all parameter were inversely identified by simultaneously using soil moisture and isotope data. Even using soil moisture and isotope data in a two step approach was better compared to using soil hydraulic parameters estimated from a pedotransfer function. The fitted flow and transport parameter were used to

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simulate and compare components of the water balance and transit time distributions yielding similar model performances.

The manuscript presents an important topic; particularly because the measurement of water isotope depths profiles in soils does not require extensive pore water extractions methods anymore. It will be a frequently used method in future, to determine integrative information about soil water flow and transport. Here, the manuscript indicates on how to get not only qualitative information out of these data, but also quantitative. The study is a novel approach and certainly is of importance for the scientific community. I have some minor to major points which have to be addressed in more detail though. In particular care needs to be taken with the interpretation of the dispersivities in the deeper soil horizon.

I am looking forward reading the revised version of the manuscript.

General Comments:

- Please emphasize that you only get information about transport (dispersivity) by using isotopes; it cannot be estimated from water content or suction data
- Why are you using deuterium contents only? What about oxygen-18? Wouldn't it add to get information about parameter uncertainty?
- 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.
- 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

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identification. Can this be further used in the forward calculations to give ranges of the calculated water balance components?

- 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?

- 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.

Specific Comments

- 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 “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.

- 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)

- 11207, ln 8-13: referring to stream flow studies in catchments is not required

- 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 modelling 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).

- 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

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causes mixing and therefore, the seasonal signal gets attenuated and after a certain time cannot be used to track water particles anymore.

- 11208, ln 18, 21: “soil hydraulic properties” rather than “soil physical” (applies to entire manuscript)

- 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

- 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?

- 11211, ln 1: I reckon the authors analysed the water and not its vapour using the equilibrium method; be more specific here

- 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

- 11211, ln 6: Water flow instead of water transport

- 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.

- 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 could be misleading

- 11213, ln 3: add “(data not shown)”; it would be even more important if the d2H/d18O

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values are similar to the individual Local Meteoric Water Line

- 11213, In 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.

- 11213, In 20: "were" instead of have been

- 11213, In 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.

- 11214, In 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

- 11214, In 14, Table 2: how were these initial parameter chosen? Were the initial parameters gained from PTFs in these ranges too?

- 11215, In 11: "(PTF)" has to be introduced here and not in In 2, 11216

- 11215, In 15-17: was an initial range for dispersivities chosen too?

- 11216, In1, 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

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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.

- 11216, In 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

- 11216, In 28: why intermediate and how were these two events chosen? arbitrarily? please be more specific

- 11217, In 22: this information (soil moisture sensors) needs to be given in the methods section

- 11220, In 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.

- 11220, In 24-25: see previous comment

- 11221, In 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.

- 11221 In 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 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 there-

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fore, it is no explanation if a PTF works in one place and not in the other place.

- 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.

- 11222 ln 14: "reasonably well"; are there any data available for comparison and to be more specific here?

- 11222 and 11223: see earlier comment about dispersivities at Hartheim and Eichstetten

- 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.

- 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

- 11223, ln 8-19: It was difficult reading this section and following your thoughts.

- 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?

- 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?

- Table 1: please add the maximum root depth in the table

- Figure 1: please change the range of the y-axis for Hartheim (e.g. 0-0.6) to better

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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)

- 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?

- 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?

- Figure 5 and 6: please indicate in the title that it refers to seepage water fluxes and transit times in 200cm depth

Interactive comment on Hydrol. Earth Syst. Sci. Discuss., 11, 11203, 2014.

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