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

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We thank the Referee 2 for the thoughtful comments and provide detailed replies in the following responses.

Comment: First, it should be made clearer what the advantages of using profiles of isotope concentrations instead of profiles of an inert tracer substance are. Especially since the measurement of isotope concentrations and the determination of the boundary conditions are much more complicated, it is important to point out the advantages of this method. In this respect, it could be useful to refer to novel experimental procedures that allow to determine these profiles online in the field ([Rothfuss et al., 2013]. Such an online method allows obtaining profiles with much higher temporal resolution,

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Discussion Paper

which might also provide important additional information that allows constraining soil parameters better.
Reply: The advantages of stable water isotopes over inert tracers either artificial introduced (Bromid, Chlorid, Uranium, Brilliant Blue) or natural tracers with regard to inverse model approaches to derive soil physical parameters are manifold. Several hydraulic processes, like infiltration, evaporation, transpiration, percolation, which take place over longer time spans are integrated in the shape of the pore water stable isotope profiles. Thus such data provides information of natural processes that happen during different hydrological states (e.g. wet or dry period). Especially, the fact that stable isotopes are part of the water molecule and therefore extracted (without fractionation) via root water uptake is a very helpful information to take for example seasonal preferential root water uptake (during summer and spring) and thus less percolation of that water into account. Such information would be hard to come by with an artificial tracer. The pore water stable isotope analysis that we use, which was originally published by Wassenaar et al. (2008), allows analyzing up to 60 soil samples a day and due to the frequent sampling of isotopes in rain, the determination of boundary conditions is not too problematic. The newly established in-situ methods presented by Rothfuss et al. (2013) and Volkamnn and Weiler (2014) will make it even more practical in future. We will include the above mentioned advantages in section 1.2 of the manuscript to clarify why we have chosen to use stable water isotopes instead of an artificial tracer.

Comment: Second, the text is at several points unclear and the methods are not sufficiently well explained. Crucial information about the measurement setup is missing in the results section it would be good to include information about the pedotransfer functions and the obtained parameters.
Reply: These points are replied in the following individual comments, where the Referee 2 has given the corresponding comment.

Comment: Third, the authors argue that they determine parameters of the soil system that are relevant for a larger scale than the scale of soil columns that are investigated

in the lab. However, I disagree with this statement since the data they use are still point data which do not have a larger support volume than the scale of lab column. This problem could be circumvented if information from many point measurements at a large number of locations is combined.
Reply: The field measurements hold information about the natural processes that happen in the field. Such conditions, as naturally developed soil structures, vegetation influences, natural time variable boundary conditions cannot or only hardly be replicated in the laboratory with soil columns. We believe to better capture these kind of processes with our field measurements of soil moisture and pore water stable isotope data. However, we agree that the soil cores are only capturing point data, but we believe that it is relative easy to measure at several locations to capture the small and larger scale variability.

Comment: Finally, I did not understand the sensitivity analysis that was carried out and I think that an uncertainty analysis of the obtained hydraulic properties and predicted seepage, annual evapotranspiration rates is necessary.
Reply: We will add a sensitivity analysis for the water balance calculation and the transit time estimations as explained in the replies to the comments by Christine Stumpp (Referee 1).

Comment: P 11205 ln12: What is meant by "transforming" water and solutes. How can water and substances be 'transformed'?
Reply: As indicated, we refer to Blum (2005), where the functions of soils are discussed. The original sentence is: "Filtering, buffering and transformation capacity between the atmosphere, the ground water and the plant cover, strongly influencing the water cycle at the earth surface, as well as the gas exchange between terrestrial and atmospheric systems and protecting the environment including human beings, against the contamination of ground water and the food chain." (Blum, 2005, section 1.1.2). Transforming is meant in a way where water is being transferred/converted between the different environmental compartments. Within these transformations, soil plays a

major role.

Comment: P 11207: ln1-2: I think that the authors misinterpreted the results of Vanderborght and Vereecken here. In figures 4 and 5 of Vanderborght and Vereecken, there is not a difference between dispersivities derived from column or field scale experiments. The important factor seems to be the transport distance. As long as the soil columns are long enough, parameters that are relevant for field conditions could also be obtained from column scale experiment.
Reply: It is true that there are no differences within the same range of the travel distances, but between the travel distances (see, Fig. 6 in Vanderborght and Vereecken, 2007). Thus, it is crucial to derive the diserpsivity parameter on the scale of interest, which would not be the case for soil cores. Therefore, we will change the sentence in a way to focus on the differences between soil cores and field data. However, Vanderborght and Vereecken (2007) state that "lateral redistribution may take place cross a larger distance so that field-scale dispersion was larger than the dispersion observed in column-scale studies. Therefore, column-scale studies in coarse-textured soils,[. . .], may not be representative for field-scale dispersion,[. . .]" (Vanderborght and Vereecken, 2007). We will include this issue in that paragraph to clarify the asset of using field data.

Comment: P 11208: ln 3-5: 'Despite the high information content of soil water isotope profiles, this type of data has so far not been included in inverse parameter identification approaches for the purpose of vadose zone modelling.' I would like to bring to the authors' attention two papers by Mathieu Javaux who analyzed chloride tracer profiles in a deep vadose zone to derive vadose zone transport parameters[Javaux and Vanclooster, 2004a; b]. The problem that was dealt with in these papers is similar to the analysis of water isotope profiles since also non-controlled variations of chloride in the input water were used to interpret time series of concentration measurements at different depths.
Reply: The studies by Javaux and Vanclooster (2004a; b) used an extremely labor and

cost intensive experimental set up, which has only little to do with the pore water extraction method that we present. We present in our study that a much easier experimental set up results in valuable information for inverse modeling approaches that include the transport parameters and not only the soil hydraulic parameters. We show that taking two to several isotope profiles, instead of generating a time series like Javaux and Vanclooster (2004a; b), is helpful to derive water flow and transport parameters. In contrast to Javaux and Vanclooster (2004a; b), we did not use porous cups to extract the water, but the direct equilibration method by Wassenaar et al. (2008), which provides tracer information of a wider pore spectrum than suction lysimeter samples with a constant suction of 80 kPa. Because of the listed differences, we don't see a lot of parallels to our study, but we will highlight the mentioned differences.

Comment: P 11208 ln 9-10: '(ii) parameter optimization/estimation should be conducted on the scale of the application.' I agree with this statement but the critical question is whether the observations represent the scale of application. If isotope concentration profiles are determined at the local scale, i.e. a small volume around a suction cup, then it is questionable whether these measurements are representative for a larger scale. The same holds true for soil water content measurements. If water contents are measured only at a single location with a sensor that has a small sampling volume (such as the 5TE sensors) then it is also questionable whether this measurement is relevant for a larger scale.
Reply: Obviously, there is the issue of the heterogeneity of the soil all soil physicists have to deal with. To account for the heterogeneity, we averaged three soil moisture sensors at each depth for the study site in Roodt. For the other sites, there were no replicate measurements available. For the pore water stable isotope profiles, there were usually only one profile taken. However, we took isotope profiles in parallel for another study and showed that the variation between the profiles can be very similar within a distance of 5 m. However, we focus in this sentence on the scale difference between laboratory measurements on soil cores compared to data taken in the field.

HESSD
11, C5812–C5820, 2014

Interactive
Comment

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Discussion Paper

Comment: P 11209: ‘slightly clayey silt’ and ‘silty sandy’: use correct nomenclature for soil texture classes. These texture classes do not exist in the USDA textural triangle.
Reply: The given expression are according to a German classification. We will change it accordingly into “silt” and “silt loam”.

Comment: P 11209: In 18-19 ‘All three sites are located on undulating terrain, where vertical flow is dominating and lateral subsurface flows can be neglected.’ Give the maximal slopes. Given that the soils are relatively shallow in the Roodt catchment, I am wondering whether the weathered schist does not lead to perched water tables and lateral subsurface flow.
Reply: We will include the information that the slope is at all the sites below 3°. At the site in Roodt, we have installed piezometers, which have never been shown any indication of a perched water table in the soil.

Comment: P 11209 ln 20- p 11210 ln 5: Which soil sensors were installed, at which depths, how many repetitions per depth how far were the soil sensors separated from each other? How many soil samples were taken to determine the water content profiles, how many profiles were taken for the isotope concentration measurements, what was the size of the cores, how far where the cores from the location of the soil moisture sensors? Part of this information is in table 1 but not everything. Table 1 should be referred to in the text.
Reply: As elaborated in the reply to Christine Stumpps comments, we will give more detailed information on these issues. A reference to Table 1 will be added.

Comment: P 11210: ln 27-29: ‘The isotopic composition of the rainfall in Roodt and Eichstetten and throughfall in Hartheim was determined at the study sites at least 14 months before the isotope profile sampling started and then at least every 14 days’ I did not understand this. Do you mean that the at least 14 months before the isotope sampling, isotope composition of rain/throughfall water was determined at least every 14 days.
Reply: Yes, that is what we wanted to say. We will reframe it as follows: “The isotopic

composition of the rainfall in Roodt and Eichstetten and throughfall in Hartheim was determined at least every 14 days at the study sites over a period of at least 14 months before the isotope profile sampling started.

Comment: P 11211: ln 1-3: 'To minimize the influence of the initial conditions of the deuterium concentration in the pore water, the time series of isotope concentration of the precipitation were extended with additional isotope data from other sampling locations close by.' I did not understand this: in what sense was the isotope concentration of precipitation 'extended'?
Reply: We have lengthened the time series with data from other locations that were close by. We will add more information on this extension, as already stated in our reply to Referee 1.

Comment: P 11214 ln 2-5: The definition of the upper boundary conditions is not precise enough. First, the upper boundary condition at the soil profile is not governed by the evapotranspiration since the evapotranspiration includes both evaporation from the soil surface and transpiration from the canopy. Second, it is not clear how the boundary condition for the Deuterium is set when evaporation occurs. I suppose that a zero concentration of Deuterium at the soil surface is set when evaporation occurs and a third type boundary condition when infiltration with a known concentration occurs.
Reply: We will change this part to clarify that the evaporation is the upper boundary and does not include the transpiration, which is a sink term in the Richards equation according to the root density. As stated in the section, the upper boundary is defined as a Cauchy type boundary conditions, which is a third-type boundary condition. The concentration of deuterium does not change due to evaporation, as stated in section 2.2.2, since we use a modified version of the HYDRUS-1D model. Thus the amount of water of a certain concentration decreases; not its concentration.

Comment: P 11216: The parameter space was not unconstrained in the other cases. It was constrained by preset ranges that were derived based on expert knowledge.
Reply: We will change that sentence from "[. . .], but unconstrained in the other

approaches,[. . .]" into "[. . .], but less constrained based on expert knowledge, [. . .]".

Comment: P 11216: I don't think that the sensitivity analysis that is presented is appropriate. Since the SCE-UA algorithm looks for the best parameter set, the distribution of the parameter sets that are obtained do not represent a posterior parameter distribution. The question is whether the distribution will become ergodic or reach a steady variance if always more and more parameter sets are considered. If this is not the case but if the distribution always becomes narrower and narrower around the optimum parameter set when more and more parameter sets are evaluated in the monte-carlo chain, then the width of the distribution depends of the number of parameter sets that were considered in the monte carlo chain. The width of the distribution of the 10
Reply: This is true and therefore, we clearly state that this sensitivity analysis is not comparable to the sensitivity analysis that are usually done with a Monte-Carlo optimization algorithm. As stated above and as already elaborated in the response to Refree 1, we will include a sensitivity analysis of the water balance calculations and the transit time estimations with several parameter sets derived during the optimization process.

Comment: P 11217 ln 1: If only two events are considered, why are the rain intensities of the events 'between' 8 and 13mm d-1 considered then? I would say that the rain intensities were 8 or 13 mm d-1. Or were several applications in different years in the beginning of October or the beginning of May considered?
Reply: We chose two events for each study site. Thus, six events were considered in total. We will change the sentence as follows for clarification: "To infer transit times through the soil profiles rain input was traced virtually at each study site for two events of intermediate intensities (between 8 and 13mmday-1), one at the beginning of October (called "fall event") and one at the beginning of May (called "spring event")."

Comment: Chapter 3.1: Simulation results using parameters derived directly from pedotransfer functions are discussed. But, I would propose to include the parameters derived from pedotransfer functions also in a table and maybe also show the hydraulic

functions that were obtained from pedotransfer functions in figure 4.
Reply: Since the simulations with the PTF do not result in a comparable good agreement as the other approaches do, we passed on a visualization of these data. We will still do so in a revised manuscript, because the additional information is limited on the cost of lucidity.

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