

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

Anonymous Referee #2

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This paper presents an interesting study on the use of water isotopes in combination with soil moisture measurements to determine soil hydraulic and transport properties. The results show that the isotope profiles provide additional information that helps to constrain better soil parameters. This is to my best knowledge the first paper in which soil hydraulic and transport properties were derived from isotope data determined in the field in combination with soil moisture measurements. The paper could be improved on a number of points. 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 experi-

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mental 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, which might also provide important additional information that allows constraining soil parameters better. 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. In the detailed list of comments, I try to give some suggestions for improvements. 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. 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.

Detailed comments:

P 11205 In12: What is meant by âĂŽtransforming' water and solutes. How can water and substances be 'transformed'? P 11207: In1-2: 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. P 11208: In 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.

P 11208 In 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.

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.

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.

P 11209 In 20- p 11210 In 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.

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P 11210: In 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.

P 11211: In 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'?

P 11214 In 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.

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.

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% best parameter sets will then depend also on the number of parameter sets that were evaluated in the Monte-Carlo chain and not only on the sensitivity of the parameter.

P 11217 In 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?

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.

References Javaux, M., and M. Vanclooster (2004a), In situ long-term chloride transport through a layered, nonsaturated subsoil. 1. Data set, interpolation methodology, and results, Vadose Zone Journal, 3(4), 1322-1330. Javaux, M., and M. Vanclooster (2004b), In situ long-term chloride transport through a layered, nonsaturated subsoil. 2. Effect of layering on solute transport processes, Vadose Zone Journal, 3(4), 1331-1339. Rothfuss, Y., H. Vereecken, and N. Brueggemann (2013), Monitoring water stable isotopic composition in soils using gas-permeable tubing and infrared laser absorption spectroscopy, Water Resources Research, 49(6), 3747-3755.

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