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Interactive comment on "EcH$_2$O-iso 1.0: Water isotopes and age tracking in a process-based, distributed ecohydrological model" *by* Sylvain Kuppel et al.

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The authors would like to thank the Referee 3 for her/his valuable comments to deepen the discussion of the conceptualisation adopted and the results. It has been taken into account in the revised manuscript and we reply point-by-point in the following (original referee's comments in bold).

This review report is for the manuscript, entitled: "ECH$_2$O-iso 1.0: Water isotopes and age tracking in a process-based distributed ecohydrological model" by Kuppel et al.. This study embedded the water isotopic tracers and age into an ecohydrological model, ECH$_2$O and then applied this model onto a small catch-

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ment. This model, therefore, could simulate the spatio-temporal variation of water flux and water isotopic composition in soil moisture, plant xylem, and groundwater. Overall speaking, I enjoyed reading this study which, indeed, is a great and innovative work. The spatio-temporal patterns of water isotopes can be demonstrated now and the hypothesis we have been concerned can be tested. The simulation is promising, which indicates that the present concepts and knowledge are tentatively correct. However, there are still some concerns that should be addressed for completing the statements.

First of all, this study simulated the hydrological processes without parameterization and calibration. Although the lack of calibration is a good way to test hypothesis comprehensively, it would lower the practical applicability for transferring this model to other catchments. This Aberdeen catchment with intensive observations is quite unique around the world. Therefore, it would be great to discuss the potential parameterization, particularly for the soil moisture, transpiration, and groundwater. The parameterization could not only increase the applicability for other catchments, but also help to introduce the landscape characteristics into the parameters, which is an important concern of critical zones where researchers attempt to incorporate the geophysical characterization into substance transport.

We appreciate this comment. We must emphasize first that the ensemble of parameters sets used for the presented simulations derives from a multi-objective calibration conducted using hydrometrics and energy balance datasets as constraints (see Sect. 3.3), following the methodology of Kuppel et al. (2018). Most likely further calibration using isotopes datasets would introduce additional independent information capable of further refining the identification of model parameters. However, we chose not to conduct such calibration in order to put the new isotope tracking model to a fundamental test: we simply assess how the original ECH_2O structure (informed by hydrometry-based parameterization and successfully evaluated) performs when applying the current “tracer tracking” conceptualization.

This first step is in our view necessary to develop a solid and hypothesis-driven contribution to the emerging velocity-celerity (i.e., looking at both hydrological response and tracer transport) modelling community, even before engaging in the provision of a ready-to-use numerical tool. Although the positive results we present are very encouraging, our “minimalistic” approach also facilitates translating the model-data mismatches into specific development needs (as discussed in Sect. 5), something which would have been challenging otherwise, given the relative complexity of the original ECH_2O model itself. We agree with the Referee that our catchment is unique in terms data availability. Hydrologists using this model in other catchments will mostly have hydrometry-related datasets available for calibration, with perhaps a few (if any) isotopic datasets. Assessing the information transferability from one viewpoint (energy celerity, provided by hydrometric datasets) to the other (water velocity as represented by isotopic composition and water ages), and their compatibility, is a reason why we did not include our isotopic datasets in the calibration.

We are nonetheless aware of the pressing need for tracer-enabled models such as ECH_2O-iso to retrieve landscape-relevant model parameterizations to leverage information-rich combinations of hydrometric and isotopic datasets. We are currently working on such a calibration approach using isotopes, along with further hypothesis-testing regarding soil mixing. We have added this aspect to the end of the revised abstract:

“[. . .] Balancing the need for basic hypothesis testing with that of improved simulations of catchment dynamics for a range of applications (e.g., plant water use under changing environmental conditions, water quality issues, and calibration-derived estimates of landscape characteristics), further works could also benefit from including isotope-based calibration.”

Secondly, the water isotopic measurement in soil moisture is very difficult and

tricky. As mentioned by Orlowski et al. (2016), it is intricate to determine the soil water isotopic composition. Presently, this model integrated all soil layers into one storage, which is acceptable, but can the authors explain more on what kind of soil water they simulated and what is their opinion about this issue in modeling work?

Finally, the observed lc-excess values of groundwater are higher than simulated ones indicating the exaggerated mixing across the soil profile. However, evaporation from shallow groundwater could raise the lc-excess variability as well. Can the authors explain more to this concern and provide some thinking for further modeling development?

We grouped the two above comments by the Referee since they are interlinked.

Being able to compare simulated soil water isotopic composition with measurement representing a similar spatial footprint is key for correct model evaluation. Currently, the soil hydrology of ECH_2O differentiates between three vertical layers in each grid cell, (whose thicknesses are calibrated parameters). Our results present the soil water isotopic composition (Figs. 3–4) of the first two layers and correspond to bulk soil water. Although we mention it in the results and discussion section (P14L17, P18L10, and P26L23), this is missing from the method section. In the revised manuscript, we have added this precision in this isotopic model description (P6L9):

"Note that because of its representation of a single, fully-mixed pool in each soil layer, ECH_2O-iso essentially provides a bulk water values for isotopic content and water ages. This needs to be kept in mind when comparing with soil isotopic datasets (see Sect. 3.2 and Sect. 4) and for the discussion (Sect. 5)."

A significant contribution of the reported model-data lc-excess discrepancy can probably be attributed to the coarse vertical discretization of the soil profile (3 layers), which enhances mixing compared to approaches that use a finer discretization of the soil profile (e.g. Sprenger et al., 2018). Overestimated mixing may be a reason for the buffered

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simulated isotopic signal and high lc-excess in the soil profile and in the groundwater.

This explanation is unsatisfying because it is rooted in the arbitrary numerical partitioning of the soil, and not on a hypothesis about hydrologic function. An alternative and more satisfying reason may be inadequacies of the full-mixing assumption and the need for a second type of water pool in each soil layer mixing at a different rate, which is a hypotheses guiding current model development. This dual mixing hypothesis relates to preferential flow pathways and is controlled by the degree of tension under which the water is held in the soil and the macro- to micro-scale variability of pore size (Beven and Germann, 2013). Despite being a long-standing issue in hydrological conceptualisation (Beven and Germann, 1982), associated efforts for catchment modelling are relatively rare and only recently gain momentum (e.g., Stump, 2007; Vogel et al., 2010; Sprenger et al., 2018; Smith et al., 2018). Without getting into the complexity (and potentially prohibitive computational cost) of applying a detailed description of a dual-porosity-based routing in the subsurface (e.g., Hutson and Wagenet, 1995) to the structure of the ECH_2O-iso model, we are currently exploring a parsimonious implementation for future studies with ECH_2O-iso. We have amended the corresponding part of Sect. 5.2 in the revised manuscript (P28L21):

"[...] dynamics and tracer mixing (Beven and Germann, 2013). This would first involve implementing conceptualisation of micro-topographic controls on overland flow (Frei et al., 2010). Secondly, the significance of sub-surface dual pore space (matrix-macropore) representations of tracer flow paths and mixing has long been put forward (Beven and Germann, 1982) but modelling efforts relevant to catchment hydrology remain somewhat scarce (Stumpp et al., 2007; Stumpp and Maloszewski, 2010; Vogel et al., 2010; Sprenger et al., 2018; Smith et al., 2018). Bridging these detailed plot-to-hillslope-scale descriptions [...]"

Finally, evaporation of shallow groundwater is not explicitly taken into account in the current ECH_2O-iso formulation of evaporative losses and isotopic fractionation. While these processes are not likely a major contributor to water fluxes and isotopic fractionation in our catchment (as hinted by the positive lc-excess values), future developments should take into account these process, which can become significant in locations with higher evaporative demand (e.g., Soylu et al., 2011).

Thirdly, the simulated and observed deuterium composition and lc-excess in forest sites exist large discrepancies. It was straightforwardly attributed to the dependency among species. It indicated that vegetation pumping has great differences among species (e.g. heather and forest). It will be great if the authors can give some suggestions for further parameterization.

The last paragraph of Sect. 5.2 (P28L19), discusses the observed model-data mismatch in Scot pine xylem and highlights limitations in our approach because: 1) we assumed soil-dependent root-profile, instead of a vegetation-dependent parameterization, and 2) unrepresented processes that could cause isotopic fractionation at different stage of xylem water cycling, e,g. during root uptake, via inner-stem exchange (e.g., xylem-phloem cycling) and via evaporation through the bark (see references in Sect. 5.2). These mechanisms are complex, non-exclusive, and the lack of a scientific consensus has made them a very active topic of ecophysiological research (Poca, *personal communication*). It is therefore difficult to suggest specific parameterization, but a first step to obtain probably requires to increase the temporal resolution of measurements and use it to derive a relationship that can be incorporated in models and that capture short-term variability (e.g., Martín-Gómez et al., 2016).

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