

Interactive comment on "EcH₂O-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 2 for her/his valuable comments and suggestions to strengthen the analysis presented in this manuscript. They have been taken into account in the revised manuscript, as follows (original referee's comments in bold):

Kuppel et al. presents a physically-based ecohydrological model ECH $_2$ O-iso that can track water isotopic tracers (2H and 18O) and age. The ECH $_2$ O-iso is an extension of the ECH $_2$ O model (Maneta and Silverman, 2013). The ECH $_2$ O-iso model was evaluated at the Bruntland Burn catchment in the Scottish Highlands, and the simulation results show reasonable agreements with the isotopic mea-

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surements. The paper is well written and structured, and it could be a potentially useful contribution to the literature. However, the authors used very general terms in many parts of their model evaluation, which makes it diffcult to assess the reliability of their results. For example, no statistics were shown on any of the time series plots, so there is no way that the readers can examine the model performance. Therefore, a major revision is suggested to improve the presentation of the current manuscript.

We thank the reviewer for this suggestion. The mean absolute error (MAE) values have been added to all relevant time series in the revised manuscript (showing the ensemble median only, so as not to overload the figures), complementing the evaluation metrics provided in summary Fig. 8. The latter has according been modified, by using normalized MAE (using each datasets range) against the Pearson's correlation factor (the revised figure can be found at the end of this doucment):

"Figure 8. Summary of model performance in the dual space of mean absolute error (normalized by the observed range of values) and Pearson's correlation factor between modelled and observed time series, for $(a)\delta^2 H$ and (b) lc-excess, showing the median and 90%-spread over the ensemble. The size of each symbol is proportional to the logarithm of the number of observation points available. Performances in soil compartments at Forest site A are further separated between periods 2013 and 2015-2016 (the latter indicated with an asterisk), corresponding to two separate field data collection campaigns. Two groundwater wells are presents at the peat site."

Additionally, we added a justification for using these metrics at the end of Sect. 3.4 (P13L26):

"As outlined in Sect. 1, our model evaluation is meant to test the ability of ECH₂O to generically simulate isotope dynamics across compartments. We used mean absolute error (MAE) to quantify model-data fit for all isotopic outputs, some of which present low temporal variability, have skewed distributions, or have a relatively lower

sampling record and resulting in typical hydrograph-oriented efficiency metrics (e.g., Nash-Sutcliffe or Kling-Gupta, Nash and Sutcliffe, 1970; Kling et al., 2012) being less applicable. The median value are shown on corresponding time series (Figs. 3–7). It is then normalized by each dataset range and used in conjunction with Pearson's correlation factor in Fig. 8 as a summary of model performance. The correlation coefficient axis in this dual model performance space represents the quality of the model in representing the variation of the data, while the normalized MAE axis provides information on the accuracy (bias) of the model."

Finally, some descriptions of results have been made more precise, especially in the abstract and conclusions. Specific changes to the manuscript are detailed in 'specific comments'.

Specific comments

Pg2, L9-12: The statement provided here seems not directly related to the paragraph above and below it. It is not clear what was the authors' attempt to deliver here. Also, what is "simplistic" meant by the authors with regard to the hydrology in land surface models?

The phrasing was awkward and has been edited for clarity. Our intent was to indicate that land surface models are the only type of process-based models operating at scales larger than the hillslope where isotope tracking has been implemented (to our knowledge). However, simplifications in the representation of hydrological pathways, such as lateral connectivity, make them of limited applicability to understand water mixing and storage dynamics. In the revised manuscript, this paragraph has been reformulated as follows:

"[...] While the simulation of energy budgets and biogeochemical cycles is increasingly

detailed in these land surface models –sometimes including vegetation dynamics–, the hydrology has, however, remained somewhat simplistic (or even absent) regarding lateral transfers as overland flow, shallow and deeper subsurface flows, and channel routing (Fan, 2015). This makes it difficult to take advantage of isotopes tracking to characterise the role of cascading downstream water redistribution in the spatial patterns of catchment functioning. [...]"

Pg3, L28-31: It is not clear how these questions being addressed in the paper. It would be very helpful if the authors could add more details about the experimental design to illustrate how these questions were linked to the results.

We have modified the end of the introduction in the revised manuscript, so that the connection between research questions (now modified following Referee #1's suggestion) and our experimental/analytical design is clear (from P3L20 onwards):

"This model was chosen because it provides a physically-based, yet computationallyefficient representation of energy-water-ecosystem couplings where intra-catchment connectivity (both vertical and lateral) can be explicitly resolved. In addition, ECH₂O separately solves the energy balance at the top of the canopy and at the soil surface, allowing a process-based separation of Es, Et, and Ec. The novel isotopic and age tracking module is designed in a fashion directly consistent with the original model structure, assuming full mixing in each model compartment, and crucially without catchmentspecific parameterization. The conceptualisation of evaporation fractionation uses the well-known Craig-Gordon approach (Craig and Gordon, 1965). We ask the following questions:

- To what extent can a hydrometrically-calibrated, physically-based hydrologic model correctly reproduce internal catchment dynamics of isotopes?
- What are the limitations of these isotopic simulations? Do they relate to the underlying model physics and/or to the tracking approach adopted?

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• How useful and transferrable is this model framework for simulating spatiotemporal patterns of isotopes and water ages?

These questions are here addressed by testing this new tracer-enhanced model (ECH₂O-iso, Sect. 2) in a small, low-energy montane catchment (Sect. 3). This site has previously been modelled applying the original ECH₂O model for calibration, using multiple datasets of long-term ecohydrological fluxes and storage variables (Kuppel et al., 2018). We take advantage of this earlier work as a reference ensemble of calibrated model parameterizations, and no additional isotopic calibration is conducted. In addition to using long-term, high resolution isotopic datasets for rainfall and runoff (²H and ¹⁸O), we assess the spatio-temporal variations of model-data agreement in soil water, groundwater, and plant xylem at different locations (Sect 4.1). Following this generic evaluation, the model is used to infer seasonally-varying patterns of water fluxes and isotopes signatures (Sect. 4.2), and water age (Sect. 4.3). Model strengths and weaknesses, insights in processes and potential ways forward are discussed in Sect. 5, before drawing conclusions in Sect. 6."

Pg4, L4: It might be better to change "climate" to "microclimate" since the spatial and temporal scales used in the model is relatively small than the scales used in climate science.

Since the model is designed to be used at a range of spatial scales, including regional studies (Simeone, 2018), in the revised manuscript we have used the term "local climate".

Pg4, L11: What is the temperature threshold for the partitioning between liquid and snow components? How does the model quantify snowpack depth for a given amount of precipitating snow?

For this threshold we use a default value of 2°C from Maneta and Silvermann (2013). Snowpack depth is not quantified in the model; only the snow water equivalent is being output by the model, and has been used for evaluation in Maneta and Silvermann

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(2013). In the revised manuscript, the corresponding section of the paragraph now reads:

"[...]. The capacity-excess P (i.e., throughfall) is partitioned between liquid and snow components using a snow-rain temperature threshold (fixed to $2^{\circ}C$) together with the minimum and maximum air temperature at each time step. [...]"

Pg4, L12: Canopy conductance is a key factor determining the amount of canopy transpiration. How is canopy conductance represented in the model? Is it simulated at each model time step?

Stomatal conductance is represented by a Jarvis-type multiplicative model to account for the four major environmental stressors driving stomatal conductance, and then upscaled to canopy conductance using the leaf area index (LAI) (Maneta and Silverman, 2013):

$$g_{canopy} = g_{stoma}^{max} \cdot LAI \cdot f_{light} \cdot f_{temp} \cdot f_{VPD} \cdot f_{\Psi}.$$

Stomatal conductance is calculated for each vegetation type in each cell of the model. Here, g_{stoma}^{max} is the maximum stomatal conductance (a calibrated parameter), while f_{light} , f_{temp} , f_{VPD} , and f_{Ψ} are efficiency factors (range 0-1), respectively, which account for the effect of incoming shortwave radiation ($R_{SW\downarrow}$), air temperature (T_a), vapor pressure deficit at the leaf-air interface ($e_a^* - e_a$), and soil matric potential (Ψ). All these variables are calculated at each time step for each vegetation type present in the grid cells, noting that f_{Ψ} is dynamically updated within the Newton-Rapson loop used to solve the 3-equations system for the canopy-level energy balance (see Appendix A1 in Kuppel et al., 2018 for further details):

$$\begin{split} f_{light} &= \frac{R_{SW\downarrow}}{R_{SW\downarrow} + \phi_{SW\downarrow}} \\ f_{temp} &= \left[\frac{T_a - T_{min}}{T_{opt} - T_{min}} \cdot \frac{T_{max} - T_a}{T_{max} - T_{opt}} \right]^{\left(\frac{T_{max} - T_{opt}}{T_{opt} - T_{min}} \right)} \\ f_{VPD} &= \exp\left[-\phi_{e_a} \cdot (e_a^* - e_a) \right] \\ f_{\Psi} &= \frac{1}{1 + \left(\frac{\Psi}{\Psi_d} \right)^c} \end{split}$$

where $\phi_{SW\downarrow}$, T_{min} , T_{opt} , T_{max} , ϕ_{e_a} , Ψ_d , and c are empirical coefficients whose values are taken from the literature ($\phi_{SW\downarrow}$, T_{min} , T_{max} , ϕ_{e_a}) or calibrated (T_{opt} , Ψ_d , and c). While adding this full description is beyond the scope of the paper, in the revised manuscript we modified the sentence highlighted for the Referee, as follows:

"The canopy energy balance then separately yields plant transpiration (E_t) and evaporation of intercepted water (E_c). The calculation of E_t uses, for each vegetation type, the canopy conductance at each time step based on a Jarvis-type multiplicative model accounting for environmental limitations of incoming solar radiation, T_a , vapor pressure deficit at the leaf surface, and soil water potential (see Maneta and Silverman (2013) and Appendices in Kuppel et al. (2018) for a more detailed description). Infiltration of surface water [...]"

Pg6, L3: Δt is redundant here as it has been defined right above eqn (2).

This redundant definition has been removed.

Pg8, L13: Could the authors provide any reference for the amount of PET estimated at the study site?

We noticed that the value reported here is an estimate of actual evapotranspiration derived from applying the Penman-Monteith equation adjusted for heather shrub aerodynamic roughness (Birkel et al., 2011). This correction, reference, and precision has been added to the revised manuscript.

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Pg11, L27-29: Were there any missing data during the measurement period? If so, what was the gap-filling treatment for the meteorological observations? Also, what was the temporal resolution of the meteorological observations?

The three weather stations at the catchment provided micrometeorological measurements at an original resolution of 15 minutes. Some measurements were sparsely missing in each of the stations records, with gaps ranging from one 15-min time step to a few days (notably during severe rainstorms at the beginning of 2016). There was however no instance of data simultaneously missing from all three stations, so that the daily inputs used for our simulations did not require a specific temporal gap-filling approach in the preprocessing stage. The revised manuscript includes information about the original temporal resolution of the raw meteorological data.

Pg 12, L 13: How did the authors determine the transient dynamics has been removed after a 3-year spin up period?

It was achieved by visual inspection of the time series of hydrometric and isotopic variables at the set of locations used in this study: through incrementing the spinup length starting from 1 to 6 years; no significant changes or trends were observed beyond 3 years of spinup. We added this precision in the revised manuscript (P12L11):

"For all simulations a 3-year spin up period was added using the first three years of isotopic and climatic model inputs, as preliminary sensitivity tests combined with a visual inspection of simulated hydrometric and isotopic time series at the locations used in this study (Sect. 3.2) indicated it was sufficient to remove transient dynamics."

Pg 12, L21: Why did the authors set the depth of the first soil layer to 0.001 m? How sensitive does the model respond to the changes in the depth of the first soil layer?

The depth of the first layer was set to 0.001 m at locations where a significant proportion (>0.5) of the grid cell area is bare soil, which always corresponds to locations with exposed bare rock. This choice was made to limit the local soil evaporation simulated by the model (which only occurs in the first soil layer and thus is strongly controlled by its depth), and avoid producing an unrealistic degree of isotopic fractionation. Sensitivity tests shows that the overall effect was small in simulating the water balance given the relatively small area covered by exposed rock, and that the isotopic composition in downstream soils and in the stream channel was barely affected by this choice of a very thin topsoil. In the revised manuscript, the corresponding sentence has been modified as follows:

"To avoid an overestimation of local soil evaporation and resulting isotopic fractionation in grid cells of exposed rock/scree, for simplicity we fixed the depth of the first soil layer to 0.001 m wherever the fraction of bare soil was larger than 0.5 – after performing a sensitivity analysis showing little effect on catchment water balance and downstream isotopic budgets."

Pg 13, L11: It should be Eq. 20 instead of Eq. 19.

It has been corrected in the revised manuscript.

Pg 19, L 26-27: How is the seasonal change of vegetation represented in the model? Was the increase of ecosystem transpiration resulted from the increase of vegetation leaf area or the increase of canopy conductance? Did the authors check the water loss from canopy evaporation? How much of difference did the model simulate between canopy evaporation and soil evaporation?

For this study, we adopted the same configuration as Kuppel et al. (2018) where vegetation dynamics is turned off, i.e. leaf area index (LAI) remains constant. As a result, the variation in ecosystem transpiration results from that of canopy conductance (see our reply about its calculation a few comments above), and that of vapor gradient at the leaf surface (see also Eq. A4 in Kuppel et al. (2018)). We have added this precision in Sect. 3.3 (P12L20) of the revised manuscript:

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"As in Kuppel et al. (2018), the dynamic vegetation allocation module is switched off, so that leaf area index remains equal to initial values of 2.9, 1.6, 3.5, and 2 m².m-2 for Scots pines, heather shrubs, peat moss and grasslands, respectively (Albrektson, 1984; Calder et al., 1984; Bond-Lamberty and Gower, 2007; Moors et al., 1998)."

The simulation ensemble provides a catchment-wide values of 354 ± 50 mm/yr for canopy evaporation (here understood as interception losses plus transpiration), which is much higher than soil evaporation (59 ± 22 mm/yr). Note that this large dominance of canopy evaporation (85-90% of the evaporative losses) over soil evaporation was also highlighted by observation-based, plot-scale studies at the same catchment in a Scots pine stand (Wang et al., 2017a) and at a heather plot (Wang et al., 2017b).

Pg29, L23: Please change "T he" to The.

It has been corrected in the revised manuscript.

Pg30, L13-14: This is a very general statement. It would be very helpful if the authors could revise it with more specific terms so the readers can catch up easily.

This is a good suggestion, and we provide more specific summary in the revised manuscript:

"Evaluated against a multi-site, extensive isotopic dataset encompassing a wide range of ecohydrological compartments (soil moisture, groundwater, plant xylem, and stream water) across hydropedological units, the model has generically shown good performance in reproducing the seasonal and higher-frequency variations of absolute and relative isotopic content (iAd'2H and lc-excess, respectively)."

Pg30, L14-15: Again, it is difficult for the readers to understand why this wound indicate the model is correct in both energy celerity and flow velocity viewpoints. It might be useful to explain what exactly are the energy celerity and flow velocity viewpoints meant by the authors.

The definition of celerity and velocity viewpoints, given in the abstract and introduction, are here repeated for clarity in the revised manuscript:

"This isotope-based evaluation suggests a correct capture of the velocity fields (i.e., how fast water parcels move) across the catchment, and complements a previous calibration and evaluation mostly using hydrometric observations (water fluxes and stores) which indicated a good simulation of catchment functioning from a celerity viewpoint (i.e., how fast energy propagates via the hydraulic gradient) (Kuppel et al., 2018). Satisfying this dual velocity-celerity perspective is key to characterizing water pathways [...]"

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Fig. 1. New Figure 8

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