General Comments R1

In this paper, the authors apply a tracer aided hydroecological model to assess the role of frozen ground on water fluxes, storage and ages in a cold regions watershed in northern Sweden. The model performed well enough to make sound conclusions about the relative magnitude of fluxes and the distribution of ages of water comprising different components of the water budget. The subject matter of this research is very relevant in regards to beginning to address larger questions about how climate, vegetation and hydrology interact. These are important questions as the globe warms, and tools such as the model introduced here will be important for predicting and attributing change. The paper is well written. I have some minor suggestions where improvements could be made. A bigger concern is an incomplete explanation of how the authors assessed the role of ground frost on water fluxes and ages. The authors explain that they turn frost dynamics off in the model to do so. I perhaps misunderstand, but how is it possible to not have the soil freeze if the same forcing dataset is used? This is a crucial piece in the methodology and it needs better explaining than currently exists. Without it, the paper does not achieve its goals. There are some suggestions I have that might improve the presentation. My specific comments are below.

Response to General Comments R1:

The authors thank Reviewer 1 (Chris Spence) for the indispensable comments which have greatly aided in the clarity of the manuscript. The primary concern raised by Reviewer 1 relates to the dynamics of the soil frost routine. The authors recognize that the explicit nature of the modifications of the model to account for long-term freezing temperatures in water physics may not have been stated as clearly as necessary. For additional clarification, the authors have revised the manuscript to state that the model would not previously freeze water (regardless of temperature) as the model was not originally designed for cold regions. The modifications presented here allow the model to account for phase change of soil water during freezing conditions as well as limit the mobility of solid water.

Major Comments

R1C1: Page 1 Line 34: It is not clear how the limited number of monitoring sites is tied to implications of hydrological change. Maybe rephrase to "The limited number of long-term monitoring sites with high quality data is a concern because it may prove difficult to document the anticipated hydrological change in these catchments".

Response to R1C1: The authors thank reviewer 1 for the suggestion, and have revised the statements (Lines 33-35, Page 1)

R1C2: Page 4 Line 39: How is the equation presented here related to the assumption that the ground and snowpack temperature are the same?

Response to R1C2: Within the model framework implemented with the freeze-thaw cycles, the surface temperature below the snowpack (T_s) is not isothermal with the snowpack or the

temperature above the snowpack. Estimations of the frost depth using isothermal estimations would result in an overestimation of the frost depth. To clarify that the soil profile and snowpack is are not isothermal the authors have adjusted the manuscript to better explain the temperature damping and thermal conduction (Lines 151 - 154, Pages 4-5).

R1C3: Page 5 Line 50: Here and elsewhere, the paper would benefit greatly from the inclusion of units when introducing variables.

Response to R1C3: The authors have revised the manuscript to include units of variables where they are introduced (e.g. Line 167, Page 5).

R1C4: Page 5 Line 50: These equations imply the soil moisture scheme assumes no movement of water in the column? I cannot think this is correct, and I must misunderstand. Could the authors please improve the clarity here?

Response to R1C4: The reviewer is correct that this is not how water movement is estimated. The change in soil water due to freezing shown with Eqn. 5 occurs after water redistributed within EcH2O. The authors have clarified the statement before the equation to indicate that redistribution occurs before the estimation of soil moisture change due to freezing (Lines 165-166, page 5).

R1C5: Equation 6: It might be the version I see, but the equation seems incomplete and the description doesn't quite match with no mention of outflow.

Response to R1C5: The authors thank the reviewer for noticing this typo. There were two subscripts missing in the equation and have been added in the revision (Eqn 6. Line 170, Page 5).

R1C6: Page 5 Line 62: Perhaps show the equation from Ala-aho, to show the difference to the reader.

Response to R1C6: The authors thank reviewer 1 for the suggestion. The authors have included the equation (inline, Line 182, Page 5) to provide a direct comparison for how the modifications are conducted and the influence of the change, as well as the physical meaning of these changes.

R1C7: Figure 1 could be better drafted and explicitly label the locations of S12 and S22. **Response to R1C7:** The authors have revised Figure 1 to include the locations of both S12 and S22 as an inset plot.

R1C8: Page 6 Line 90: Not all of this section includes model data, and some is observational data. You could perhaps retitle the section "Observations".

Response to R1C8: The authors have revised the title of the section to "Input and calibration datasets" (Line 213, Page 7).

R1C9: Page 7 Line 20: Perhaps put the simulation period right at the beginning of the section.

Response to R1C9: The authors have moved the statement of the periods of the simulation to the beginning of the section (Lines 241 - 243, Page 8).

R1C10: Figure 2: Could the authors add a sentence or two explaining why the water ages bottom out every now and then? Perhaps I have missed it.

Response to R1C10: The water ages in the stream drop suddenly due to rain on snow events which result in rapid runoff of young water rapidly mixing with the older stream water. The relatively low streamflow volume during the winter months results in a large influence in the stream water ages. This explanation has been added to the manuscript (Lines 301 - 303, Page 10).

R1C11: Page 10 Line 89: Are the words dynamic and damped mixed up? **Response to R1C11:** The authors have revised the wording (Lines 313 – 314, Page 11).

R1C12: Figure 3: Please explain what 'normalized' means.

Response to R1C12: The authors have added the description to the manuscript (Line 268, Page 9) and within the figure (Line 325, Page 10).

R1C13: Figure 3: Also, why does the soil water age get younger as the summer progress? The paper would benefit from a few sentences explaining this behaviour.

Response to R1C13: The soil water age decreased during the summer due to the flushing of older snowmelt and pre-winter water, replaced by younger growing season precipitation. Unlike many other studies, snowmelt age is accumulated throughout the winter months, and snowmelt is not input to catchment storage with an age of 0 days. The authors have added a statement to explain the decrease in soil water ages during the summer (Lines 319 - 320, Page 11).

R1C14: Figure 5: Just so apples are compared to apples, perhaps total modelled evaporation and transpiration so that it can be more easily compared to the ICOS data.

Response to R1C14: The authors have added the simulated ET to Figure 5d to directly compare to the ICOS tower ET (Fig. 5, Page 13).

R1C15: Page 13 Line 41: A citation might be useful here because the data from this paper do not support such a statement.

Response to R1C15: The authors have removed the statement from the manuscript.

R1C16: Page 15 Line 88: The authors have access to soil temperature data that could show if this is underestimated. A figure might help address this gap. Also, please explain how the assumption of no temperature gradient through the snowpack influence these results **Response to R1C16:** The authors have clarified in the manuscript (Line 115, Page 3) that the soil temperature is only estimated at one location in the soil domain (the interface of the first and

second thermal layers). Similar to Response to R1C2, there is a diffusive gradient of temperature through the snowpack estimated with a calibration parameter (Line 154, Page 5). The authors have also added some discussion on potential over-estimation of heat sink (under-estimation of thermal conduction) to the discussion (Lines 416 - 418, Page 15).

R1C17: Page 15 Line 93 - 99: There are some typos through this section that could be fixed. **Response to R1C17:** The authors have revised this section to improve the grammar and typos (Lines 424 - 430, page 15).

R1C18: Page 16 Line 27: I missed where the ages of the soil frost are provided. It would be valuable to show them.

Response to R1C18: The authors have revised Figure 3 to include the water ages of soil frost (Page 11).

R1C19: Page 16 Line 30: It would be helpful to provide data on the relative values of these fluxes and storages in the text here to let the reader know how important each is to determining the age of water.

Response to R1C19: The authors thank the reviewer for the suggestion. The authors have provided numerical values in-line to aid the reader in understanding how the mixing and timing of different water sources will influence the water ages (Lines 468 – 469, Page 16).

R1C20: Page 16 Line 32: Maybe rephrase to "...of older soil frost with younger soil water and snowmelt reduces....."

Response to R1C20: The authors have revised the statement using the reviewer's suggestion (Lines 470 – 471, Page 16).

R1C21: Page 16 Line 35: Was it limited or just hard to detect within the uncertainties of the model? This is an important point of discussion that is missing.

Response to R1C21: There is a combined effect of model uncertainty and limited effect. On the smaller streams, the influence of the soil-frost on the stream water age is more apparent, with younger snowmelt reaching the stream faster due to overland runoff as with rain on snow (limited infiltration). In some model parameterizations the differences are apparent in all streams; however, on average, these differences are not significant when compared to the model uncertainties of water ages. The authors have added this to the discussion section (Lines .432 – 436, Page 15).

R1C22: Page 16 Line 43: I am not convinced the results of the research support these statements. Please clarify. If more water is pulled from soil subject to warming would not that speed up the pattern observed in Figure 3? And in turn reduce age?

Response to R1C22: The authors have revised this statement to clarify that the increase in water availability (regardless of vegetation) will result in higher water use of the younger water in the soils. Higher use of younger water for vegetation results in less young water feeding the groundwater and stream, thereby increasing the water ages (Lines 478 – 482, Page 16).

General Comments of Reviewer 2

The paper by Smith et al., seeks to use a previously developed ecohydrological model (EcH2Oiso) to further understand the partitioning, water storage, flux and age inter-actions, particularly in the context of cold, northern catchments. This novelty of this contribution is that they have adapted the model to include soil freezing, and the impact of soil freezing on water ages. As the authors note, most model estimations of storage-flux interactions oversimplify vegetation-soilwater interactions, while EcH2O-iso provides a generic and relatively simplistic (in some parts) modeling approach to evaluate storage and water ages in cold environments. The model of course has limitations related to the process physics and the assumption of complete isotope mixing within each compartment, which may not hold true. However, the authors are transparent as to its shortcomings in most places, and it is of little value to be overly picky with regards to the choices that are made. The manuscript is well written, and the figures are clear and of high quality. I would like the authors to consider the comments below and I believe the manuscript is suitable for publication after minor revisions. The main conclusion of the work is that soil frost had an early season influence on the ages of transpiration, with less of an influence on water ages of evaporation. Second, that the new module can simulate soil frost dynamics. While I do not dispute this, it is unsurprising that the Stefan-type of equations can simulate frost well, this approach has been used for ages and ages and while perhaps not always a physical realistic representation of ground freezing, it simply works well (as it does here). It would be good for the authors to indicate whey they did not use a more complex thermal scheme, or reference ones. Obviously, one would need more soil layers and computational resources would go through the roof, but a bit more on the 'why' this method was used is good. I would like to focus my comments around the central conclusion re: soil frost and water ages. It would be useful to outline how evaporation and transpiration are partitioned as this would help the reader (although it is likely presented elsewhere) and goes to the central conclusion.

Response to General Comments of Reviewer 2

The authors thank reviewer 2 for their constructive comments for the manuscript. The choice here for using the relatively simple Stefan's equation to solve for the soil frost depth because the authors were trying to minimize the changes to the model structure of EcH2O. The authors had explored more comprehensive thermal schemes, the current model structure of EcH2O resolves the energy balance at the surface through an iterative approach and would not allow for a simple adaptation of the model structure. Changes to the model structure would significant alter the energy balance of the surface (and also the canopy). This would be an interesting development but would need additional testing in both the winter and summer conditions to ensure that there is not a significant error with a different energy balance estimation. Additional estimation methods of soil frost have been added to the introduction section. The authors have added further descriptions of how the evaporation and transpiration are estimated in the model description section.

Major Comments

R2C1: Equation 1 simulates the depth of the freezing front, but not the soil temperature. I am curious as to how the model simulates soil temperature. I THINK I understand how the surface temperature is driven, and the authors acknowledge that the thermal routine of the snowpack is simple for various reasons. What I'm trying to get at is: does the model simulate a soil temperature and how does this relate to the position of the zero-degree isotherm. Yes, soils will be identified as frozen or unfrozen base on Eq1, yet is there a modeled soil temperature that simply has no freezing routine? More clarity is needed.

Response to R2C1: The model does estimate a soil temperature; however, the implementation of soil temperature was derived for warm climates where there are not discontinuities with the thermal conductivity or heat capacity (due to ice conditions). These discontinuities influence the depth that the soil temperature is recorded as there is no soil temperature profile estimated within the model framework so it is not currently possible to identify the zero-degree isotherm in the model. There is additional work to be conducted with the model to account for the ground heat flux under the snowpack, with may require a more robust thermal diffusion through the snowpack to properly estimate the soil temperatures. The authors have clarified the estimation of the soil temperatures when introducing the energy balance of EcH_2O (Lines 112- 117, Page 3).

R2C2: The central conclusion that soil freezing affects transpiration is fine, but is it simply because the plants are not 'on' when the soil is frozen and soil evaporation is impeded (it certainly would be). When the module is off, plants can transpire, and soils evaporate? Is it this simple? I'm just not sure. More clarity on what drives the transpiration would be helpful as I'm unsure if there can be no transpiration when the rooting zone is frozen – how does this all work? **Response to R2C2:** The authors have clarified this in the discussion section. The soil frost does not turn 'on' or 'off' the transpiration or soil evaporation, rather, the soil frost restricts the water available for transpiration. As transpiration is a function of the water available, the transpiration and thereby isn't restricted to the same degree (Lines 458 - 461, Page 16).

R2C3: Is there sublimation in the model? I see that latent heat is set at 0 when there is snow – why? What impact does this have when snow is melting and sublimation maybe important. **Response to R2C3:** There is not currently a sublimation module from the snowpack surface within EcH₂O (latent heat set to 0). However, there is some sublimation from the canopy interception, though there is not currently a phase dependent interception within the model (SWE and rainfall depths have the same interception capacity in vegetation). This may have some effect on the water volumes during the spring months and increase the dominance of the soil frost conditions. A brief section to the discussion section has been added about the influence of sublimation (Lines 414 - 422, page 15).

R2C4: For Equation 7, what is the basis of the amplification factor C. Does equation 7 pre-serve an isotope mass balance throughout all time steps (I'm assuming so – but it should be stated). **Response to R2C4:** The authors recognize that the meaning of C was not provided in the manuscript. While S is representative of the shape of the snowmelt fractionation curve (i.e. timing of the melt), the amplification factor is representative of the atmospheric effect on the fractionation (i.e. RH and temperature effect). To minimize "moving parts" in the model, this was held constant and calibrated. The manuscript has been revised to define C and describe the definition of Eq 7 (Lines 187 - 193, Page 6)

R2C5: The authors use ERA-Interim data to drive the radiative component of the model. For a few years, there was overlap. Did they investigate the bias of the ERA data and correct? I'm assuming ERA-I would work well in this location of Europe, but it's good to check as it can have biases which will propagate through the energy balance calculations. The underestimation in net radiation is a bit concerning – and latent heat as well. So after all this, my question is that if latent heat is in fact greater than simulated, what influence would this have on the age estimates (if any?). I assume some and this should be noted.

Response to R2C5: The authors have added a discussion on the influence of the use of the ERAdata within the study and how this may influence the results in the study. The authors did examine the difference between the ERA data to the on-site data and there is no noticeable bias with the ERA data at the site (Lines 418 - 422, Page 15)

R2C6: On line 79, I'm not sure that the CRHM reference is correct and the Xie and Gough paper describes the thermal routine that is later incorporated into CRHM (see papers by Krogh for example). The XG method is in CRHM, but this is just slightly incorrect referencing. **Response to R2C6:** The authors have revised this reference (Line 403, Page 14).

R2C7: The discussion after line 85 is a bit selective and there are dozens of possible reasons for model errors in turbulent fluxes. First the authors state sensible heat fluxes are underestimated but only show latent fluxes so the discussion should be there or sensible heat data should be provided. Another reason not stated (and noted above) is the nature of the ERA-I data. I'm also unsure as to how snow processes are incorporated into the canopy module re: unloading, albedo change, etc. All I'm saying is that there are many many reasons here where the model could be improved with physics, and avoid suggesting 'direct calibration' is the best way to improve simulations.

Response to R2C7: The sensible and latent heat fluxes (with the net radiation) are all provided on Figure 5 (rather than just latent heat). It was not the intention of the authors to state that "direct calibration" was the only means to improve the estimation of the heat flux estimation, rather that some of the model parameters may be sensitive to the heat flux that were not included in the calibration because the heat flux (evaporation or transpiration either for that matter) were not calibrated. Thereby, any inclusion of those parameters would yield not significant posterior distribution. The authors have modified this section to indicate that there are multiple processes (some of which are not yet included in the model) that may influence the energy balance while stating that the potential reasons are examples of influences (Lines 411 - 422, Page 15).

R2C8: Figures that highlight the differences between soil moisture at depth would be helpful. **Response to R2C8:** The authors chose to not include the soil moisture at depth since the model was not directly calibrated to different soil moisture depths, and showing this dataset may result in confusion that the model was calibrated to distinct soil depths. This calibration was not directly possible due to the calibration of soil layer depths 1 and 2 which limited the comparability of the calibration with variable depths. The soil moisture at different depths have been added to the appendix for additional information for the readers.

Specific Comments

R2C9: Line 80: under different vegetation communities (forest vs mire). 2) To examine the influence of soil frost on the dynamics and age of water (Comma instead of period after(forest vs mire)

Response to R2C9: The authors have revised this typo (Line 85, Page 3)..

R2C10: Line 54: qin \rightarrow subscript needs to be added **Response to R2C10:** The authors have revised this typo (Eq 6, Page 5).

R2C11: Line 73: comma needed within coordinates **Response to R2C11:** The authors have revised this typo (Line 196, Page 6).

R2C12: Line 95: "Stable isotopes determinations were carried out" \rightarrow Fix wording **Response to R2C12:** The authors have revised this wording (Line 218, Page 7).

R2C13: Table 1: Units of precipitation say $m/s \rightarrow$ should be moved to wind speed. Units need to be added to other dat. "30 min for Sensible Heat says " 30 in". Column heading needs to say "Time Period" for top row.

Response to R2C13: The authors have revised this table to include units for all input and calibration /validation data (Table 1, Page 7).

R2C14: Line 69: stream isotopes tended to retain a slight "memory" effect from the more enriched late summer..."contributions"? "water"? I think a word is needed here? **Response to R2C14:** The authors have revised this statement (Line 292, Page 10).

R2C15: Beginning Line 95: While some work has been conducted on assessing the transit or residence times of ecohydrologic fluxes or their partitioning in northern (e.g. Sprenger et al., 2018a); however, few studies have included the influence of frozen conditions on the water

movement, which may be significant for the effective transit times during the spring freshet period (Tetzlaff et al., 2018) and flow path modelling in "cold" regions(Laudon et al., 2007; Sterte et al., 2018).

Response to R2C15: The authors have revised this statement (lines 427 – 430, Page 15).

R2C16: Line 99: Traditionally, water ages in stream water at catchment outlets have been the primary metrics for assessing the transport of tracers. Should this read: Traditionally, isotopic tracers in stream water at catchment outlets have been the primary metrics for assessing water ages.

Response to R2C16: The authors have revised the statement (Line 430, Page 15).

R2C17: Line 29: snow and early spring snowmelt), and snowpack is the amount "weighed" age of solid precipitation (*Should this be weighted)

Response to R2C17: The authors have revised this typo (Line 467, Page 16).

Assessing the influence of soil freeze-thaw cycles on catchment water storage – flux – age interactions using a tracer-aided ecohydrological model

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11

12 Abstract

13 Ecohydrological models are powerful tools to quantify the effects that independent fluxes may have on catchment storage 14 dynamics. Here, we adapted the tracer-aided ecohydrological model, EcH2O-iso, for cold regions with the explicit 15 conceptualisation of dynamic soil freeze-thaw processes. We tested the model at the data-rich Krycklan site in northern Sweden 16 with multi-criteria calibration using discharge, stream isotopes and soil moisture in 3 nested catchments. We utilized the model's 17 incorporation of ecohydrological partitioning to evaluate the effect of soil frost on evaporation and transpiration water ages, and 18 thereby the age of source waters. The simulation of stream discharge, isotopes, and soil moisture variability captured the seasonal 19 dynamics at all three stream sites and both soil sites, with notable reductions in discharge and soil moisture during the winter 20 months due to the development of the frost front. Stream isotope simulations reproduced the response to the isotopically-depleted 21 pulse of spring snowmelt. The soil frost dynamics adequately captured the spatial differences in the freezing-front throughout the 22 winter period, despite no direct calibration of soil frost to measured soil temperature. The simulated soil frost indicated a maximum 23 freeze-depth of 0.25 m below forest vegetation. Water ages of evaporation and transpiration reflect the influence of snowmelt-24 inputs, with a high proclivity of old water (pre-winter storage) at the beginning of the growing season and a mix of snowmelt and 25 precipitation (young water) toward the end of the summer. Soil frost had an early season influence of the transpiration water ages, 26 with water pre-dating the snowpack mainly sustaining vegetation at the start of the growing season. Given the long-term expected 27 change in the energy-balance of northern climates, the approach presented provides a framework for quantifying the interactions 28 of ecohydrological fluxes and waters stored in the soil and understanding how these may be impacted in future.

29 1. Introduction

30 Northern watersheds are sensitive hydrologic sites where a significant proportion of the annual water balance is controlled by the spring melt period (Kundzewicz et al., 2007) and can thus be key sentinels for detecting climate change impacts (Woo, 31 32 2013). Recent data and long-term climate projections indicate a significant increase in warming for extensive areas of boreal forests 33 currently experiencing low-energy, low-precipitation hydroclimatic regimes (Pearson et al., 2013). The limited number of long-34 term monitoring sites with high-quality data is a concern because it may prove difficult to document the anticipated hydrological 35 change in these catchments (Laudon et al., 2018; Tetzlaff et al., 2015). Within changing northern catchments, with high water loss 36 due to transpiration (~48 ± 13%) (Schlesinger and Jasechko, 2014), and significant influence of evapotranspiration (ET) fluxes on 37 streamflow (Karlsen et al., 2016a), the long-term ecohydrological implications of vegetation adaptation, plant water use, and the

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42 water sources that sustain growth are crucial to understand and quantify. Vegetation in boreal regions also exerts strong influences 43 on the energy balance of such catchments, with low leaf area index (LAI) conifer forests and shrubs affecting the surface albedo, 44 snow interception and affecting the timing and duration of the largest input fluxes of water during snowmelt (Gray and Male, 45 1981). However, the interactions between soil water storage and "green water" fluxes of transpiration and evaporation are poorly 46 constrained in northern regions, and the way in which sources of water from inputs of snowmelt and summer rainfall mix and 47 sustain plant growth is only just beginning to be understood (Sprenger et al., 2018a). Assessment of these interactions in northern 48 catchments is further complicated by large temperature variations, and the resulting stagnation of hydrological processes induced 49 by frequent frozen ground conditions. With increasing temperatures and potential changes to the winter soil freeze-thaw dynamics 50 (e.g. Venäläinen et al., 2001), it is important to establish how these affect current vegetation-soil water interactions to project the 51 implications of future change

52 The intricate complexities of changes in the land surface energy balance, temporal changes in sub-surface storage due to frost 53 conditions, and vegetation and soil water usage (transpiration and soil evaporation, respectively), are notoriously challenging to 54 continuously monitor (Maxwell et al., 2019), particularly in northern environments, where site access is typically remote and 55 extreme cold can limit in-situ monitoring devices. In these circumstances, the fusion of sparsely available data with hydrological 56 models is an effective method to quantify water fluxes and storage dynamics at different temporal and spatial scales. While the 57 calibration of such models requires significant hydrometric data inputs, recent work has shown that incorporation of stable isotopes 58 can be an effective tool for constraining the model estimations of storage - flux interactions in the absence of direct in-situ 59 measurements. Such models include (but are not limited to); the STARR (Spatially distributed Tracer-Aided Rainfall-Runoff) 60 model (van Huijgevoort et al., 2016), which was developed for tracer-aided simulations and calibration, and adapted for additional 61 cold-regions processes (Ala Aho et al., 2017a and b; Piovano et al., 2018), CRHM (Cold Regions Hydrologic Model) specific for cold regions (Pomeroy et al., 2007), but not currently using tracers, the isoWATFLOOD model (Stadnyk et al., 2013), which has 62 63 been used to isolate water fluxes with tracer-aided modelling in large-scale applications in northern regions of Canada, and the 64 EcH₂O-iso model (Maneta and Silverman, 2013; Kuppel et al., 2018 a and b), which was developed as a process-based, coupled 65 atmosphere-vegetation-soil energy balance ecohydrologic model, and modified to incorporate isotopic tracers (stable isotopes deuterium and oxygen-18, δ^2 H and δ^{18} O, respectively). However, apart from EcH₂O-iso, which explicitly conceptualises short-66 67 term (diurnal and seasonal) and long-term (growth-related) vegetation dynamics and biomass productivity, most of these existing 68 models were mainly developed with a focus on runoff generation ("blue water" fluxes). Consequently, they have very simplistic 69 representation of vegetation - soil - water interactions, estimating ET by approximating the physical transpiration controls of vegetation (e.g. Penman-Monteith and Priestley-Taylor methods) and partitioning fluxes after estimation of actual ET (Fatichi et 70 71 al., 2016).

72 Currently, EcH2O-iso, already incorporates some cold region processes, namely snowpack development, a snowmelt routine, 73 and the influence of temperature effects on vegetation productivity. While the depth of the snowpack is not directly estimated (only 74 snow water equivalent is tracked), the surface energy balance incorporates snowpack heat storage to estimate the warming phase 75 with effective snowmelt timing (Maneta and Silverman, 2013). The model additionally estimates soil temperature, however, 76 freezing temperature and soil frost development are adaptations that are needed for use in catchments with extensive freezing 77 conditions. Soil freeze-thaw has the potential to significantly influence soil moisture conditions, tracer dynamics, and the 78 magnitude and ages of all water fluxes. Soil freeze-thaw cycles have been estimated with a variety of methods, ranging from the 79 Stefan equation (i.e. cumulative freezing temperatures) to the more physically based Richards-Fourier calculations (e.g. Zhang et 80 al., 2007; Zhang et al., 2011). The simplicity of the Stefan equation is useful in many circumstances, including where computational

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83 efficiency is important (as in with EcH2O-iso) which restricts the use of small time and space steps of physically based models. 84 Additionally, the Stefan equation works well in most environments when soil latent heat is much larger than the sensible heat, and 85 there are linear gradients of soil temperature (Jumikis, 1977). The incorporation of tracer dynamics to EcH2O-iso open 86 opportunities to strengthen the evaluation of the model processes (Kuppel et al., 2018b) and permits the use of tracers in calibration 87 (Douinot et al., 2019). Here, our overall aim was to provide a framework for assessing vegetation influences on the hydrology of cold-regions by adapting the EcH2O-iso model and testing it in the intensively monitored Krycklan catchment in northern Sweden. 88 89 The specific objectives of the study are three-fold; 1) to assess the capability of a spatially distributed, physically-based 90 ecohydrological model to capture the influence of snow and soil freeze-thaw processes on water storage dynamics, and the resulting 91 flux magnitudes under different vegetation communities (forest vs mire), 2) To examine the influence of soil frost on the dynamics 92 and age of water fluxes within the catchment, and 3) provide a generic modelling approach for application to other frost affected 93 catchments. In the adaptation of EcH2O-iso to cold regions and the assessment of the simulated vegetation-soil water interactions

94 with frost conditions, we aim to improve the understanding and projecting the future role of vegetation in cold regions hydrology.

95 2. Model description and extensions for this paper

96 2.1 EcH₂O-iso model

97 Recent advances in hydrological modelling have included more explicit process-based conceptualisation of ecohydrological 98 interactions (Fatichi et al., 2016) and the integration of tracer-based data (Birkel and Soulsby, 2015). The EcH₂O model (Maneta 99 and Silverman, 2013) was developed as an ecohydrological model coupling land-surface energy balance models with a physically-90 based hydrologic model. This explicitly includes the dynamics of vegetation growth and vertical and lateral ecohydrological 91 exchanges.

02 2.1.1 EcH₂O energy balance

03 The energy balance is computed for two-layers, the canopy, and surface. The solution of the energy balance is used to calculate the available energy reapportionment for transpiration, interception evaporation, soil evaporation, snowmelt, ground heat storage, 04 05 and canopy and soil temperature. The canopy energy balance is iteratively solved at each time step until canopy temperature 06 converges to the estimated value that balances radiative (incoming and outgoing short and long wave radiation), and turbulent 07 energy fluxes (sensible and latent heat) (Maneta and Silverman, 2013; Kuppel et al., 2018 a and b). Long- and shortwave radiation 08 transmitted through the canopy to the soil and longwave radiation emitted by the canopy toward the ground drive the surface 09 energy balance. The surface energy balance components include radiative exchanges (incoming and outgoing short and long-wave 10 radiation), sensible, latent, and ground heat fluxes, as well as heat storage in the soil and in the snowpack. Soil evaporation is 11 estimated with the latent heat, using the atmospheric conditions (air density and heat capacity), soil resistance to evaporation, and 12 the aerodynamic resistance (surface and canopy) of the evaporative surface (Maneta and Silverman, 2013). The transpiration is 13 estimated at the leaf and is dependent on the vapour pressure gradient from the leaf to the atmosphere, the canopy resistance to 14 vapour transport, vegetation properties, and the current soil saturation conditions (Maneta and Silverman, 2013). While the energy 15 balance apportions energy to each storage (i.e. soil and snowpack), when the snowpack is present, estimated surface temperatures 16 refer to the snowpack surface, and the surface temperature of the ground is assumed to be at the temperature of the snowpack, which means that conductive heat transfer between soil and snowpack is 0 (no thermal gradient). Also, when the snowpack is 17 present latent heat for surface evaporation is set to 0. When no snowpack is present, the ground heat flux (and soil temperature) is 18 19 estimated with the one-dimensional (1D) diffusion equation with two thermal layers, where the bottom of the top thermal layer is 20 estimated with the thermal conductivity and heat capacity of the thermal layer (Maneta and Silverman, 2013). The 1D diffusion

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23 equation is only used during the snow-free conditions since soil frost causes discontinuities in the estimation of the thermal layers.

24 While soil temperature is estimated within EcH₂O (at the interface of the first and second soil thermal layer), there is currently not

25 <u>a freezing-routine for soil water below 0°C.</u>

26 2.1.2 EcH₂O-iso tracer and water age module

27 EcH₂O has previously been adapted to incorporate the tracking of hydrological tracers including stable isotopes (Kuppel et 28 al., 2018b) and chloride (Douinot et al., submitted), and adapted to compute estimations of water age in water storage and fluxes. 29 Isotopic fractionation is simulated in soil water using the Craig-Gordon model (Craig and Gordon, 1965), and tracer mixing is simulated using an implicit first-order finite difference scheme. Full details of the implementation of the isotopic module are in 30 31 Kuppel et al., (2018a). These adaptations do not consider fractionation of snowmelt or open water evaporation. Water ages are 32 estimated assuming complete mixing in each water storage compartment. Similar to other snowmelt tracer models (eg. Ala-aho et 33 al., 2017a), the snowmelt ages are defined as the time the snow enters the catchment, rather than the time of melt. This results in 34 older water estimations during the freshet period and a more complete estimate of the time that water has resided in the catchment.

35 2.2 Soil water freeze-thaw adaptation

Hydrology in cold regions can be greatly affected by the freeze-thaw cycles of soil water during the winter, resulting in reduced liquid water storage capacity during the spring melt and a restricted capability for infiltration due to the expansion of ice in pore spaces (Jansson, 1998). The depth of the soil frost can have a large influence on the timing of snowmelt runoff and provide an estimation of the liquid water available within a soil layer (Carey and Woo, 2005). The Stefan equation is a simple energy balance approach to estimate the progression of soil water freezing (Jumikis, 1977):

$$\Delta z_f = \left[\frac{2k_f (T_s - T_f)}{\lambda \theta}\right]^{1/2} \tag{1}$$

41 where $\Delta z_{f}(\mathbf{m})$ is the change in depth of the frost and is a function of the thermal conductivity of the frozen soil layers between the 42 frost depth and the soil surface ($k_f, W \cdot m^{-1} \cdot C^{-1}$), the soil surface temperature <u>below the snowpack</u> ($T_{s_c} \circ C$), the temperature of freezing 43 $(T_{f_{0}}C)$, the latent heat of freezing (λ , J·m³), and the liquid soil moisture (θ , m³·m³). As with previous approaches (Jumikis, 1977; 44 Carey and Woo, 2005), the progression of the soil frost is estimated by discretizing the total soil depth into smaller layers. Within 45 EcH2O-iso, the sub-surface soil regime is discretized into three soil layers, layer 1 (near the surface), layer 2, and layer 3 (groundwater to bedrock), to resolve the water balance and estimate soil moisture. Here, the depths of layer 1, 2, and 3 were used 46 47 as the layers since they intrinsically incorporate the soil moisture estimations without additional parameterisation. The thermal 48 conductivity of frost affected layers is dependent on the moisture content of the soil:

$$k_f(i) = \left(k_{sat} - k_{dry}\right) \cdot \left(\frac{\theta(i)}{\phi(i)}\right) + k_{dry}$$
⁽²⁾

49 where $k_f(i)$ (W·m⁻¹·C⁻¹) is the thermal conductivity of frozen soil in layer *i*, k_{sat} (W·m⁻¹·C⁻¹) is the thermal conductivity of saturated 50 soil, k_{dry} (W·m⁻¹·C⁻¹) is the thermal conductivity of dry soil, $\theta(i)$ (m³·m⁻³) is the soil moisture in layer *i*, and $\phi(i)$ (m³·m⁻³) is the soil 51 porosity in layer *i*. The saturated thermal conductivity was estimated from the proportions of soil comprised of ice, liquid water, 52 air, organic material, and mineral soil (Carey and Woo, 2005):

$$k_{sat} = \prod_{n=1}^{5} k(j)^{f(j)}$$
(3)

53 where *j* is the thermal conductivity of each volume proportion, *f* is the fraction of total soil volume, and *k* is the thermal

54 conductivity of volume *j*. Without proportions of soil organic and mineral material, the bulk soil thermal conductivity (k_{dry}) is

55	considered the weighted average of organic and mineral thermal conductivity (only 4 total volumes in Eqn 3). Implementation of		
56	Eqns 1-3 for freezing layers below the ground surface are ideal for EcH ₂ O as the model estimates the parameters (T_s , and θ) or		
57	includes parameterisation of physical properties (λ , k_{dry} , ϕ , k_{water} , k_{air}), and only requires the addition of the thermal conductivity		
58	of ice (2-1 W·m ⁻¹ ·C ⁻¹ , Waite et al., 2006). Within EcH ₂ O, the estimation of surface temperature (above the snowpack) is assumed	\leq	Deleted: 1W/
59	to be isothermal with the snowpack and conduction through the snowpack is not considered. However, <u>conduction through</u>	-(Deleted: /ºC
60	snowpack is important for the Stefan equation (Eqn 1) as the surface temperature used is below the snowpack which is generally		Deleted: within the Stefan equation (Eqn 1) is the surface
61	thermally insulated by the snowpack. To address the conduction through the snowpack without snow depth or density, the	(temperature
62	estimated surface temperature <u>above the snowpack</u> (T_{Est}) was damped with a single unitless parameter (D) such that $T_s = T_{Est}D$.		
63	To account for the reduction of the infiltration rate due to ice, models have previously adjusted the soil hydraulic conductivity		
64	(e.g. Jansson, 1998). Here, the reduction in hydraulic conductivity is estimated using an exponential function:		
	$K_{wf} = 10^{fc \cdot F} K_{sat} \tag{4}$		
65	where $K_{wf}(\underline{\mathbf{m}\cdot \mathbf{s}^{-1}})$ is the hydraulic conductivity of the soil influenced by ice, $K_{sat}(\underline{\mathbf{m}\cdot \mathbf{s}^{-1}})$ is the saturated hydraulic conductivity of		
66	ice-free soils, fc is a unitless ice-impedance parameter, and F is the fraction of frost depth to total soil depth. Equation (4) has two		Deleted: an
67	key assumptions: no ice lenses or frost heaving, and no soil volume expansion due to lower ice density (assumed <u>920 kg</u> /m ³ at ice		Deleted: 920kg
68	temperature 0-5°C).		
69	2.3 Soil frost volume, depth, and water age		
70	As soil frost progresses through the layers, the proportion of liquid water is assumed to decrease at the same rate as the		
71	proportion of unfrozen soil. Similar to other approaches estimating the moisture content of frost-affected soils (Jansson, 1998), a		
72	minimum liquid soil moisture was retained in all frozen soils. This minimum was assumed to be the residual soil moisture (θ_r),		
73	the minimum moisture content required for evaporation and root-uptake. Following the estimation of the soil water infiltration		Deleted: The
74	and redistribution of soil water within EcH2O, the change in soil moisture due to freezing in each layer is estimated:		Deleted: of
1	$\Delta\theta = (\theta(i) - \theta_r) \cdot \frac{\Delta z_f}{d(i) - d_r(i)} $ ⁽⁵⁾		
75	where $\Delta \theta (\underline{m^3 \cdot m^{-3}})$ is the change in liquid water and ice content, $\theta(i) (\underline{m^3 \cdot m^{-3}})$ is the initial liquid content in layer i, $\theta_r (\underline{m^3 \cdot m^{-3}})$ is		
76	the residual moisture content, $d(i)$ (m) is the total depth of layer i, and $d_F(i)$ (m) is the depth of frost in layer i. Step-wise		Formatted: Font: Not Italic
77	estimation of freeze and thaw for each layer is provided in more detail in Appendix A. The water age of the ice is estimated in a		
78	similar way to the liquid water ages of the soil layers (Kuppel et al., 2018b):		
	$V_{res}^{t+\Delta t} A_{res}^{t+\Delta t} - V_{res}^{t} A_{res}^{t} = \frac{1}{\sqrt{q_{in}}} A_{in}^{t+\Delta t} - q_{out} A_{res}^{t+\Delta t} $ (6)		Deleted: $q A^{t+\Delta t}$
79	where t is time (sec), Δt is the time-step (sec), V_{res} (m ³) is the volume of ice in storage, q_{in} (m ³) is the volume of water from the		Deleted:
80	change in soil moisture during freeze-up (using $\Delta \theta$ in Eqn 5), q _{out} (m ³) is the volume of water from the change in soil moisture		Deleted: ,
81	during thaw (from. Eqn 5), and A (sec) is the water age (subscripts res and in are the water ages in storage and inflow, respectively).		Deleted: from
82	Similar to the isotope and vegetation modules in EcH2O, the frost dynamics (i.e. frost depths and water ages) were implemented		
83	as an option within EcH ₂ O.		
84	2.4 Isotope snowmelt fractionation		
85	Isotopic fractionation of snowmelt can have a significant influence on the composition of streams (Ala-aho et al., 2018a).		
86	Previous successful applications of a simple approach equation to estimate the isotopic fractionation of snowmelt at multiple		
87	locations has shown that low-parameterised fractionation models can be used to spatially approximate snowmelt fractionation. One		
88	of the noted limitations of the simple snowmelt fractionation approach used in Ala-aho et al., (2018a), is the dependence of the		Deleted: 2018
89	snowmelt fractionation on the past snowmelt volumes (total days of melt, d_{melt}) rather than current snowmelt rate $d\delta^2 H_{melt}$ =		Deleted: .

04 $\delta^2 H_{pack} - M_{frac}/d_{melt}$, M_{frac} is a fractionation parameter, in Ala-aho et al., 2018a). The approach was modified to include the 05 snowmelt rate with one additional parameter using an exponential function:

$$\delta^{2}H_{melt} = \delta^{2}H_{pack} - \left(S \cdot exp\left(-S \cdot \left(1 - \frac{SWE - M}{SWE_{max}}\right)\right)\right) \cdot C$$

.06 where $\delta^2 H_{melt}$ (‰) is the isotopic composition of the snowmelt, $\delta^2 H_{pack}$ (‰) is the composition of the snowpack at the beginning 07 of the time-step, SWE (m) is the snow water equivalent at the current time, SWE_{max} (m) is the maximum snow water equivalent 08 before melt, M (m) is the total depth of snowmelt in the current time-step, S is a unitless slope parameter describing the shape of .09 the exponential change of the snowmelt fractionation, and $C_{(\infty)}$ is an amplification factor. Eq. (7) serves as the mass-balance for 10 the snowpack isotopes throughout the winter and spring melt period. In comparison to Ala-aho et al (2018a), the exponential form 11 works to temporally change the shape of the fractionation as a relationship to the amount of melt (i.e. replacing 1/d_{melt}). Higher 12 values of S (10-20) result in larger early melt fractionation and limited late melt fractionation, while low values of S result in a 13 lower, but more consistent fractionation throughout the melt period. The amplification factor behaves as a simplification of 14 atmospheric effects on the snowmelt fractionation. The isotopic composition of the snowpack is updated at the end of each time-15 step.

16 3. Data and study site

17 3.1 Study site

18 Svartberget (C7, 0.49 km²) is a small subcatchment situated in the headwaters of the Krycklan catchment (64°14'N, 19°46'E) 19 in northern Sweden. Svartberget is a well-studied site with long-term data collection including: streamflow (1991-present), stream 20 chemistry (2000-present), and hillslope transect measurements (soil moisture and water chemistry). Svartberget has two 21 subcatchments, Västrabäcken (C2, 0.12 km²) and Mire (C4, 0.18 km²) (Fig. 1). The topographic relief of C7 is 71 m (235 - 306 m 22 a.s.l.), with 57 m of relief in C2 (247 - 304 m a.s.l.) and only 26 m of relief in C4 (280 - 306 m a.s.l.) (Fig 1). The climate is subarctic (in the Köppen classification index), with annual precipitation of 614 mm, evapotranspiration (ET) of 303 mm, mean 23 24 relative humidity of 82 %, and a 30 year mean annual temperature of 1.8 °C (Laudon et al., 2013). The relatively low topography 25 results in no observable influence of elevation on precipitation (Karlsen et al., 2016b). The catchment experiences continuous 26 snowpack development throughout the winter, accounting for approximately a third of the annual precipitation and lasting on 27 average 167 days (Laudon and Löfvenius, 2016). The large quantity of snowfall results in a dominant snowmelt-driven freshet 28 period (Karlsen et al., 2016a). Till (10-15 m thick) covers the majority of the downstream catchment area (C7, 92% downstream 29 of C4) with intermittent shallow soils in the headwaters of C2 (Fig. 1a). The catchment is predominantly forest covered (82% total, 30 98% downstream of C4), with Scots Pine (Pinus sylvestris), Norway Spruce (Picea abies), and Birch (Betula spp.). The Mire (Fig 31 1b) is dominated by Sphagnum mosses.

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(7)





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Resolution

Location

Air Temperature	Svartberg	Daily	2005-2016			
(minimum maximum and	~					
mean) (°C)						
Precipitation (m:s-1)	Svartberg	Daily	2005-2016		(Deleted: /
Wind speed (m·s ⁻¹)	Svartberg	Daily	2005-2016		×	
Relative Humidity (%)	Svartberg	Daily	2005-2016			
Longwave Radiation (W·m ⁻²)	ERA-interim	Daily	2005-2016			Deleted: interm
Shortwave Radiation (W·m ⁻²)	ERA- <u>interim</u>	Daily	2005-2016			Deleted: interm
δ^2 H Precipitation (%)	Svartberg	Event-based	2005-2016			
Calibration and Validation	Datasets					
	Location	Resolution	Time-Period			
	C7	Hourly	2005 - 2016			
Discharge $(m3 \cdot s^{-1})$	C2	Hourly	2005 - 2016			
	C4	Hourly	2005 - 2016			
	C7	Biweekly	2005 - 2016			
Stream isotopes (%)	C2	Biweekly	2005 - 2016			
	C4	Biweekly	2005 - 2016			
	S12	Hourly at depth of 5, 10, 20, 30, 40, 60 cm	2013 - 2016			
Son Moisture (IIIS-III-)	S22	Hourly at depth of 6, 12, 20, 50, 60, 90 cm	2013 - 2016			
Validation Only Datasets						
	Location	Resolution	Time-Period			
Soil Isotopes (Lysimeter	S12	9 samples: 10, 20, 30, 40, 60, and 70 cm	2012		(Deleted:)
<u>‰)</u>	S22	9 samples: 10, 20, 35, 50, 75, and 90 cm	2012			
Soil Isotopes (Bulk Water	S12		2015 - 2016			Deleted:)
<u>‰)</u>	S22	7 samples: 10, 20, 30, 40, 60, and 70 cm	2015 - 2016			
Soil Temperature (°C)		30 min @ 4 locations at depths 5, 10, 15, 30, and 50				
		cm				
Net Radiation (W·m ⁻²)	ICOS Tower	30 min	2014 - 2015			
Latent Heat (W·m ⁻²)		30 min				
Sensible Heat (W·m ⁻²)		30 min		-		Deleted: in

62 3.2.3 Soil moisture and isotope datasets

Soil moisture sensors were installed in 1997 and replaced at the beginning for 2013. The soil moisture sensors were installed 63 at the hillslope transect location at 4, 12, 22, and 28 m locations from the C2 stream. The depths of the soil moisture measurements 64 65 slightly differ between sites (Table 1); however, the depths encompass shallow and deep soil waters. Soil sensors have also been 66 installed in the area surrounding the ICOS tower, measuring soil temperature at 4 locations and 6 depths (10, 20, 30, 40, 60, and 67 70 cm, <u>Appendix B</u>) (Table 1) which can provide a proxy for the depth of the frost. Soil isotopes (δ^{2} H and δ^{18} O) were measured at 68 multiple depths (2.5 cm increments) measured via lysimeters (2012) and bulk water samples (2015 - 2016).

3.3 Model set-up and calibration 69

:70 All simulations were conducted on a daily time-step between January 2005 and September 2016. The period from January 71 2005 to December 2009 was used as a spin-up period with measured hydrologic data, to stabilize $\delta^2 H$, $\delta^{18}O$ composition, and water 72 ages in each of the model storage units. Initial analysis of the measured discharge from 2000-2016 revealed the highest and lowest 73 annual discharge years were between 2010 and 2014. Consequently, calibration was carried out for the period between January 74 2010 and December 2014. The validation set used was the remaining period from January 2015 - September 2016. The C7 75 catchment was defined with a grid resolution of 25×25 m² to balance adequate differentiation of multiple locations on the soil 76 water transect while maintaining computational efficiency. The 25 m grid includes adjacent soil pixels for S12 and S22, with sites 77 S04 and S28 within the same grids as S12 and S22, respectively. Within the biomass module, the vegetation dynamics for leaf Moved down [1]: The C7 catchment was defined with a grid resolution of 25 × 25 m² to balance adequate differentiation of multiple locations on the soil water transect while maintaining computational efficiency. The 25 m grid includes adjacent soil pixels for S12 and S22, with sites S04 and S28

within the same grids as S12 and S22, respectively.

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growth and carbon allocation were held at steady state to minimize the parameterisation and focus on the soil freeze-thaw cycles. As temperature effects and water stress are less sensitive for conifer trees, a relatively constant leaf area index and needle growth/decay rate were maintained (Liu et al., 2018). Evaporative soil water fractionation was activated using similar parameterisation to Kuppel et al. (2018b), as this has previously been identified as an influential summer process in the catchment (Ala-aho et al., 2017a). Soil relative humidity was estimated using Lee and Pielke's (1992) approach, and values of kinematic diffusion were estimated as presented by Vogt (1976) (0.9877 and 0.9859 for H²/H¹ and O¹⁸/O¹⁶ ratios, respectively). Parameterisation of the model was conducted for each soil type (3 soil types, Fig 1a) and vegetation type (4 types, Fig 1b).

97A sensitivity analysis established the most sensitive parameters to be used in calibration using the Morris sensitivity analysis98(Soheir et al., 2014). Parameters were assessed using 10 trajectories using a radial step for evaluating the parameter space. The99parameter sensitivity was evaluated using the mean absolute error. Results of this are shown in Appendix C. Sensitive parameters00were calibrated using Latin Hypercube sampling (McKay et al., 1979) with 150,000 parameter sets and a Monte Carlo simulation

01 approach to optimize the testing of the model parameter space.

02 3.4 Model evaluation

The model output was constrained using measurements of stream discharge (3 sites, Fig. 1), stream $\delta^2 H$ (3 sites, Fig. 1), and 03 04 soil moisture (2 sites, Fig. 1a). The 8 measurement datasets were combined into a multi-criteria calibration objective function using 05 the mean absolute error (MAE) with the cumulative distribution functions (CDFs) of the model goodness-of-fit (GOF) (Ala-aho 06 et al., 2017a; Kuppel et al., 2018 a and b). The MAE moderated over-calibration of peak flow events, typical for functions like the 07 root mean square error, and Nash-Sutcliffe efficiency, as well as being consistent with previous studies in the region (Ala-aho et 08 al., 2017a). To focus on the dynamics of soil moisture, given the coarse model grid, measured and simulated values were -09 standardized by their respective mean values prior to analysis. From the CDF method, the 30 "best" simulations were selected for 10 evaluation and are presented using 95% spread of predictive uncertainty (Kuppel et al., 2018b). The parameters achieved through 11 calibration are shown in Appendix D. Model results were verified against the remaining years of discharge, soil moisture, and 12 stream flow $\delta^2 H$, as well as independent time series of soil isotopes (bulk and lysimeter), net radiation, sensible heat, latent heat, 13 and frost depth (estimated from depth-dependent soil temperatures). 14 The evaluation of changes to water ages due to soil frost was conducted by comparing the ages within the catchment for 15 simulations of the 30 "best" parameter sets with and without frost. These were conducted without frost by turning frost dynamics

off within the model. Freeze-thaw effects on evaporation and transpiration ages were evaluated as the difference between frost and non-frost simulations. Positive values indicate older water with the frost while negative values indicate older water with frost-free simulations. The age differences were only considered on days when both frost and non-frost simulations simulate a flux greater than 0 mm/day.

20 4. Results

21 4.1 Simulation results

Calibration captured dynamics of both high and low flow discharge periods through both the calibration period (2010 - 2014)and validation period (2015 - 2016), with a maximum mean stream flow MAE of 2×10^{-3} m³/s for C7, and a maximum mean stream δ^2 H MAE of 5.8 ‰ at C4 (Table 2). Due to extreme high and low flow periods in the calibration period, it was unsurprising that the resulting MAE was higher than in the validation. The MAE of the soil moisture calibration was also reasonable, with average MAE of 0.05 and 0.09 for sites S12 and S22, respectively. With the <u>standardization</u> of the soil moisture, the low MAE indicates that the dynamics in the model correspond well to those measured. The optimization of the GOF for 3 measures (discharge, stream Deleted: B

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32 δ2H, and soil moisture) at 8 locations resulted in a compromise for all streams. Simulations yielded better (lower) MAE for

33 discharge and isotopes of individual streams.

Table 2: Calibration and validation efficiency criteria, shown as mean efficiency for all multi-calibration criteria 34

		Calibration (2010 - 2014)	Validation (2015 - 2016)
	Site	MAE	MAE
	C7	2×10 ⁻³ m ³ /s	6×10 ⁻⁴ m ³ /s
Discharge	C2	1×10 ⁻³ m ³ /s	1×10 ⁻⁴ m ³ /s
	C4	1×10 ⁻³ m ³ /s	3×10 ⁻⁴ m ³ /s
	C7	4.8 ‰	4.0 ‰
$\delta^2 H$	C2	4.6 ‰	3.8 ‰
	C4	5.8 ‰	3.9 ‰
Soil Moisture	S12	0.05	0.09
Soli Moisture	S22	0.09	0.09
Latent Heat	ICOS Tower	N/A	13.1 W/m ²
Sensible Heat	ICOS Tower	N/A	29.5 W/m ²
Net Radiation	ICOS Tower	N/A	31.0 W/m ²
Soil Frost Depth	ICOS Tower	N/A	0.03 m

35

Temporal variability of δ^2 H in each of the streams was captured quite well throughout the calibration and validation periods (Fig 2 a - c). The largest offsets in modelled isotopic composition occurred during the winter low flow conditions. The simulated 36 37 stream isotopes tended to retain a slight "memory" effect from the contributions of more enriched inflow in late summer. This was likely due to the underestimation of discharge during winter (Fig 2 d - f) which slowed the flushing of the more enriched water. 38 39 Overall though, discharge was adequately simulated for each site, notably during the spring melt and summer months. While flows 40 were underestimated during the winter, the difference between simulations and measurements were typically $< 1 \times 10^{-3}$ m³/s. The 41 weight-median water ages of each of the three streams were broadly similar, 2.8, 2.6, and 3.1 years for C7, C2, and C4, respectively 42 (Fig 2 g-i). These stream ages were generally older than previous estimates, with deeper soil layers and complete mixing in each 43 compartment tending to increase the average age. The depth of the soil layers in the peat and podzolic areas are the primary drivers 44 for water age, with a ~1:1 relationship (Appendix E). Water age decreased during the annual freshet, driven by the younger 45 snowmelt and frozen soil water ages (typically 150 - 200 days old). The rapid runoff during the freshet limited the long-term influence of the younger water ages on the stream water at each of the sites as older groundwater dominated low flows. Rain on 46 47 snow events resulted in some rapid, yet un-sustained, influences on the soil water ages, as observed with the sudden decreases in 48 stream water age during winter months (Fig 2 g-i; log-scale with lower bound of 250 days).

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Figure 2: Calibration 95% maximum and 5% minimum bounds, median simulation (solid line), and measured data (black circles) of δ^2 H for (a) C7, (b) C2, and (c) C4; discharge for (d) C7, (e), C2, and (f) C4; and stream water age for (g) C7, (h) C2, and (i) C4.

53 4.2 Soil moisture, isotope, and water ages

54 Simulated soil water isotopes (note that the model did not use isotopes during calibration) mostly captured those measured in 55 both bulk water (2015 - 2016) and lysimeter water (2012) within the 90% simulation bounds at the S12 and S22 sites (Fig 3 a & 56 b). Isotope dynamics were best captured at site S12, with early season depletion due to snowmelt and enrichment of the previous 57 summer. While most variability was captured within the 90% bounds, the magnitude of the intra-annual contrasts at site S22 was 58 not fully reproduced. Similar to the soil isotopes, dynamics of simulated soil moisture (calibrated) were captured at both S12 and 59 S22, with better simulation performance at S12 (Fig 3 c & d). The model struggled to simultaneously reproduce the more damped 60 soil moisture at S12 with the relatively dynamic soil moisture post-melt at S22 in the adjacent cell under the same soil 61 parameterisation. Rather, the same parameterisation resulted in balancing the conditions observed at S12 and S22. The large declines in measured soil moisture during the winter months were captured with the soil frost module (Fig 3 c & d). The modelled 62 63 decline in the soil moisture resulted from the transition of soil water from liquid to ice. Water ages in layers 1 and 2 at each site showed noticeable intra-annual variability, and gradually declined during the growing season (May - September) and increased 64 65 during the winter due to negligible water inflow (Fig 3 e & f). The gradual decrease in the soil water age during the summer was 66 the result of younger rainfall flushing the older snowmelt and pre-winter soil water as the growing season progressed. The 67 variability of the soil water ages in layers 1 and 2 was similar, though the ages in layer 2 were significantly older. While S12 is 68 closer to the stream, water ages in S22 were generally older in both layers 1 and 2.

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soil frost for (e) site S12, and (f) site S22.4.3 Soil freeze-thaw simulations

76 Simulations of frost depth revealed large inter-annual variability throughout the catchment (Fig 4 a-d), depending on winter 77 temperatures, snowpack depth, and the soil moisture conditions. Wetter conditions in the mire generally show shallower frost 78 depths than the podzolic soils elsewhere in the catchment. Similar soil conditions for the podzolic and thin podzolic soils (Fig 1a) 79 resulted in negligible differences for estimated frost depth. Overall, estimated frost depth was generally limited by the total number 80 of freezing days. Colder winters (larger numbers of freezing degree days) resulted in deeper frost depths for an equivalent snowpack 81 depth (e.g. Fig 4a vs Fig 4c). Conversely, a deeper snowpack (higher maximum SWE) resulted in a shallower simulated frost depth 82 for years with similar temperatures (e.g. Fig 4 a vs c) as the deeper snowpack was a larger storage for incoming radiation. Using 83 0°C in the soil temperature probes at the ICOS tower as a proxy for the depth of the soil frost, a direct comparison of simulated 84 frost depth and the measured catchment frost depth was completed without calibration. Simulated frost depth showed good 85 agreement with observed 0°C soil temperature depth, imitating the rapid increase in frost depth in 2014 and a more gradual increase 86 in 2015 (Fig 4e). Late winter soil frost depth was estimated to be shallower and varied more rapidly than the observed 0°C soil 87 temperature depth (Fig 4e). The median estimated soil depth against the measured 0° C soil temperature depth showed that estimate 88 soil thaw was too rapid, and thaw completed too early.

12



92 93 94 95

Figure 4: Mean simulated soil frost depth during the peak soil frost depth in winter (a) 2010-2011, (b) 2011-2012, (c) 2012-2013, and (d) 2013-2014. 90% uncertainty bounds of the simulated frost depth at the ICOS Tower with the depth of the 0°C soil temperature measured at the ICOS Tower (black circles)

96 4.4 Evaporation and transpiration

97 While the evaporation, transpiration, and energy balance datasets were not included in the calibration, modelled energy balance 98 components (sensible heat, latent heat, and net radiation) showed reasonable agreement to observed values in 2014-2016 at the 99 ICOS Tower. There was an <u>underestimation</u> of net radiation and sensible heat throughout the growing season (Fig 5 b & c), and 00 an underestimation of latent heat late in the year (Fig 5a). While the MAE of the latent heat was relatively small (13.1 W/m²) 01 considering that they were not used for calibration, net radiation and sensible heat had a notable maximum bias (\sim 30 W/m²) during 02 summer. Simulations of total daily evaporation (soil and interception) and transpiration had a similar pattern, with transpiration -03 accounting, on average, for 54% of total evapotranspiration. Throughout the year, the simulated proportion of transpiration to total evapotranspiration ranged from 31 - 72% except for the spring periods (Fig 5d). The late onset of evaporation resulted from the 04 -05 assumption that soil evaporation was negligible while the snowpack remains, which potentially lead to an underestimation of -06 evaporation during the melt.

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Figure 5: Energy balance component of (a) estimated latent heat (90% and mean values), (b) estimated net radiation (90% and median values), (c) estimated sensible heat (90% and median values) and (d) estimated soil evaporation<u>transpiration<u>and</u> evapotranspiration<u>(ET)</u> (90% and mean values), at the ICOS Tower site with the estimated total evapotranspiration from energy fluxes at the ICOS Tower (black circles where data are available).</u>

Ages of soil evaporation and transpiration decreased throughout the year (Fig 6 a and b), tracing the decline in soil water ages estimated with the addition of precipitation (age of 0 days). Older water present in evaporation and transpiration water at the start of the year was a mixture of the snowmelt water age and frozen water ages (from the previous summer). Spatial differences in evaporation and transpiration ages were evident throughout the catchment; shown by the difference between the forested ICOS tower site (blue, Fig 6 a & b), and the average for shrubs in the mire (green, Fig 6 a & b). The annual flux-weighted median water age of transpiration was 200 ± 42 and 141 ± 40 days for the ICOS tower and mire, respectively, while evaporation ages were $48 \pm$ 11 and 85 ± 36 days for the ICOS tower and mire, respectively.

21 Differences between the evaporation and transpiration ages were determined by comparing water ages with the soil frost 22 module activated, against those with the frost module deactivated. Generally, including frost in the simulations resulted in older water (water age difference > 0 Fig 6c) for both evaporation and transpiration. Differences in evaporation age were not as 23 -24 pronounced as transpiration ages due to the slight bias of the evaporation timing (always following the snowmelt). Due to the 25 estimated completion of soil thaw prior to the snowmelt period, the difference between the water ages of evaporation with the influence of frozen ground was modest. Rapid flushing of the soil water due to large snowmelt inputs and spring precipitation -26 27 resulted in a rapid decline in the differences of transpiration water ages. Within the first month of transpiration, the difference for the frost and non-frost simulations were more notable and approached 200 days when frost limited water movement. However, the -28 -29 relatively lower transpiration rates, which occurred during the spring within these simulations, resulted in a moderate effect on the -30 overall annual transpiration water ages. The effects of soil frost on stream water ages showed little effect, with negligible 31 differences given the relatively old water bias in the stream that only shows some flashes of younger water influence (Fig 2 g-i). -32 While the soil frost increased the stream water ages throughout the year, the effect is well within the relatively large uncertainty .33 bounds of the stream water ages.

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Figure 6: 90% bounds and median values of the (a) estimated soil evaporation water ages at the ICOS Tower (blue) and in the Mire (green), (b) estimated transpiration water age at the ICOS Tower (blue) and in the Mire (green), and (c) mean difference of evaporation and transpiration water ages when soil frost is not considered.

45 **5. Discussion**

46 5.1 Modelling soil freeze-thaw processes in tracer-aided models

47 Hydrologic models are powerful tools for exploring the internal functioning of catchments, particularly when intensive and 48 long-term monitoring programs are in place to help calibration and testing (Maxwell et al., 2019). Here, the development of a 49 spatially distributed, process-based tracer-aided model for northern climates produced encouraging results reproducing soil frost .50 dynamics despite the model not being directly calibrated to match frost depths observations. The use of streamflows, stream -51 isotope ratios and soil moisture dynamics in calibration proved to be adequate for estimating the dynamics of soil frost depth and timing of the frost onset (Fig 4) and revealed spatial differences in frost depth due to contrasting soil types and moisture -52 -53 conditions. However, there are limitations with the current approach that results in some uncertainty of the effect of soil freeze--54 thaw on catchment hydrology. To improve the computational efficiency of the model, the temperature of the snowpack was -55 assumed to be isothermal (Maneta and Silverman, 2013), and modified here to include only a single temperature damping parameter. However, snowpacks may have a variable thermal gradient (e.g. Filippa et al., 2014), and is dependent on snow -56 .57 density (e.g. Riche and Schneebeli, 2013), snow surface albedo, wind speed, and liquid water component, among others -58 (USACE, 1956; Meløysund et al., 2007; Sturm et al., 2010). While these additional components may contribute to an -59 improvement in the estimation of soil frost, it likely would not have a significant improvement compared to the simple temperature damping used here with additional calibration to constrain snow water equivalent for more dynamic energy 60 exchange (e.g. Lindström et al, 2002). The simplistic consideration of negligible soil sensible heat storage effects on the soil 61 -62 freeze/thaw processes, consistent with other process-based cold region models (e.g. CHRM, Krogh and Pomeroy, 2018), may 63 result in dampened rates of freezing and rapid melting during the spring (Kurylyk and Hayashi, 2016). More delayed melting of 64 the soil frost may have implications for snowmelt runoff, increasing the dynamics of the streamflow isotopic compositions

65 towards more depleted isotopic compositions (Fig 2 a-c). Finally, the simplification of a single soil frost front may have some

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68 implications for the snowmelt infiltration to the soil. The single front does not allow for near-surface soil thaw to occur prior to 69 deeper soils and thereby has implications for shallow root-water uptake and evaporation. .70 Energy fluxes in northern catchments can be highly sensitive to the timing of snowmelt, yielding differences in the surface and canopy net radiation due to changing albedo and to turbulent fluxes due to alterations in surface temperature. Here, the under-71 72 estimated sensible heat flux during the spring and the growing season could be the result of many different processes. Some of 73 these processes include the aerodynamic resistance (ra) to transpiration, an underestimated thermal gradient between the simulated soil and air temperature, an overestimation of the incoming short- or long-wave radiation from the ERA-interim dataset, 74 .75 sublimation and snowpack energy storage, or an over estimation of a heat sink of ground heat through the thermal layers of the 76 soil. An overestimated aerodynamic resistance can simultaneously reduce the transpiration (increases the surface temperature), as .77 well as decreases the sensible heat flux (Maneta and Silverman, 2013). An over estimated surface temperature can result in both a 78 decreased thermal gradient from the soil to the air used for the sensible heat flux estimation, as well as result in the shallower, and earlier, simulated soil frost melt relative to the measured 0°C soil temperature depth. While the short- and long-wave radiation .79 .80 from the ERA-interim dataset had no consistent deviation from the shorter measured time-series at the ICOS Tower (1:1 ratio for 81 both short- and long-wave radiation, not shown), intermittent periods of under-estimated ERA-interim radiation could contribute

82 an underestimation of the net and sensible heat flux. Lastly, the lack of snowpack heat storage and sublimation could have an

83 influence on the energy balance by limiting incoming winter radiation into the soils (i.e. decreasing soil temperatures).

84 5.2 Effect of soil freeze-thaw on water ages and implications for northern catchments

85 The adaptation here of a process-based, spatially distributed model to additionally incorporate fundamental cold regions processes provides both the opportunity to improve the representation of key hydrologic functions of cold catchments, and assess 86 87 the effect that these processes have on transit times and ages of ecohydrological fluxes. While studies in northern catchments have -88 aimed to assess the partitioning and transit or residence times of ecohydrologic fluxes (e.g. Sprenger et al., 2018a), few studies 89 have included the influence of frozen conditions on the water movement, Frozen conditions may be significant for the effective .90 transit times during the spring freshet period (Tetzlaff et al., 2018) and flow path modelling (Laudon et al., 2007; Sterte et al., 91 2018). Traditionally, isotopic tracers water at catchment outlets have been the primary metrics for assessing the water ages in .92 streams. Here, the relatively old age of stream water, and the underestimation of soil-thaw result in only slightly older water ages .93 when soil frost conditions are considered, potentially due to the smaller proportion of wetland areas (Sterte et al., 2018). The .94 limited effect of soil frost effects on stream water age was compounded from both the wide uncertainty of the stream water ages .95 (Fig 2g-i), and the late winter deviation of soil water frost ages from the soil water (Fig 3e & f). Generally, the uncertainty bounds 96 of the stream water ages were greater than the difference of the soil water and soil frost ages. The smaller different of soil water .97 and soil frost ages thereby resulted in small effective changes in stream water age. The deeper frost depth in the forested regions .98 likely did not reduce the spring infiltration due to the low moisture content in the soil relative to the more saturated wetlands .99 (Laudon et al., 2007). Additionally, the relatively wide uncertainty bounds of stream water age estimates present difficulties in 00 assessing the relatively moderate effects of soil frost on the stream water age (Fig 2). The large dependence of the flows and stream water ages at C7 on the outlet of the large mire at C4 indicates that the water age progressing through the mire will be a strong 01 02 determinant of long-term change. The flux-weighted median water age estimations for the streams here were estimated to be 03 substantially older than other tracer-aided hydrologic models for the catchment (Ala aho et al., 2017a), though were on the upper 04 end of other stream and hillslope transit times from transit time methods (Peralta-Tapia et al., 2016; Ameli et al., 2017). The reasons 05 for this are largely three-fold. Firstly, the model was calibrated with soil depths comparable to those observed in the catchment. 06 The calibrated model used soil depths ranging from 1.5 - 6 m, where the shallower soil depths yield stream water ages are

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Deleted: While improved timing of the soil-thaw period would likely improve this, direct calibration of the sensible heat fluxes using the vegetation and soil albedo are likely more effective routes to improved simulations.

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comparable to previous studies. Secondly, the complete mixing assumption within the model does not allow for rapid preferential movement of young water that has been observed in numerous other recent studies (e.g. Botter et al., 2010; Harman 2015). Incomplete mixing within the model framework would allow for deeper soil profiles to yield younger water fluxes, as estimated from isotopes alone, albeit at the expense of additional parameterisation. Lastly, the previous transit time estimations (Peralta-Tapia et al., 2016; Ameli et al., 2017) do not account for older water ages of the snowpack, or the immobility and aging of frozen soil water, which would increase the estimated water ages.

34 Unlike stream or soil water ages, low uncertainty of transpiration and soil evaporation ages helps bring new understanding to 35 how soil frost affects the source contributions of these ecohydrological fluxes which were the focus of the study. Ages of both 36 transpiration and soil evaporation are consistent with soil profile modelling conducted in the region using the SWIS model 37 (Sprenger et al., 2018b). However, the dynamics of the age variation are notably different due to the differences in the input water, 38 where the snowmelt input to the SWIS model assumes a water age of 0 days and does not account for the "green" water fluxes 39 during the spring months. While the transpiration ages show notable differences when frost, and the corresponding discontinuity 40 of transit times, is included in the simulation, the evaporation water ages are not greatly affected. Transpiration fluxes are 41 influenced by the frost due to the reduced liquid soil water availability and increased soil resistance to transpiration. The higher 42 soil water deficit for transpiration does not fully restrict the transpiration flux, but reduces the fluxes until soil frost thaws and 43 mixes the older frost water in the upper soil layers. The differences are reduced for both fluxes due to a few potential reasons. 44 Firstly, the timing of the soil thaw has a significant influence on age estimation of soil water available for both evaporation and 45 root-uptake. While the general timing and magnitude of the soil frost depth development seems appropriately captured by the 46 model, even without calibration, soil thaw in late winter was simulated faster than observations (Fig 4e). There are notable 47 differences between the ages of soil water, soil frost, and the snowpack, where soil frost is representative of the previous fall soil 48 water, soil water is a younger water mix of the fall soil water and newer precipitation (e.g. from rain-on-snow and early spring 49 snowmelt), and snowpack is the amount weighted age of solid precipitation. Here, shallower soil frost and early melting of soil 50 frost in the spring results in step-wise mixing, firstly of soil frost (oldest water, e.g. 200 - 300 days in Fig 3) and soil water 51 (moderate age, e.g. 100 - 125 days in Fig 3), then of the soil water mixture and snowmelt (youngest water, e.g. 70 - 90 days). 52 Since evaporation, and its corresponding age, only begins following the end of snowmelt, the greater degree of older soil frost with 53 the younger soil water and snowmelt reduces the influence of the soil frost on the evaporation ages. Delaying the simulated timing 54 of soil thaw would result in a larger influence of the soil water ages on both the evaporation and root-uptake. 55 While the influence of soil frost on stream water ages was limited in this catchment, the results have potentially significant 56 implications for modelling other catchments with frozen soils. The effect on water ages will likely be the greatest in catchments 57 where winter precipitation is limited, allowing the soil frost depth to increase from the surface, delaying the soil thaw until after 58 the primary snowmelt. For evaporation and transpiration water ages, notable spatial differences highlight an essential consideration 59 for northern climates in the influence of vegetation-type on the source of water fluxes. In many northern areas, past glaciation 60 results in significant wetlands typically dominated with shrub and herbaceous vegetation. Reductions in soil frost will result in 61 greater water availability throughout the year, aiding in vegetation growth (Woo, 2013). With increased water availability 62 throughout the year, the water use of yegetation will likely increase, and thereby limit the amount of young water percolating 63 through the rooting zone. A reduction in the amount of young water percolating through the rooting-zone will likely increase the 64 age of soil water and catchment outflows. Finally, the timing of the evaporation and root-uptake needs to be strongly considered, 65 at both seasonal and diurnal time scales. Soil frost had a strong influence on the timing of evaporation and transpiration, where the magnitude of both fluxes was greater in simulations without soil frost and timing of the root-uptake and soil evaporation was 66

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delayed due to ice-restricted pore spaces. While such changes are anticipated, many studies have focused on plot scale studies and with estimated long-term reductions of soil frost depth, larger scale estimations of these differences are essential to understanding how catchment ecosystems will respond.

80 6. Conclusion

In northern environments, with a rapidly changing climate, quantitative evaluation of vegetation interactions with catchment 81 82 soil water is crucial for understanding and projecting catchment responses. The process-based evaluation here of a well-monitored, 83 long-term study catchment in the northern boreal forest region using a tracer-aided, surface-atmosphere energy-balance model has 84 provided significant insights into the importance of soil freeze-thaw processes. Tracers were used, not only as a calibration tool, but as validation metrics, and highlighted the effectiveness multi-criteria calibration of a model at nested scales using discharge, 85 isotopes, and soil moisture to constrain additional, un-measured, features (e.g. soil frost depth). The progressively younger ages of 86 87 evaporation and transpiration throughout the growing season show the dependence of both "green water" fluxes on spring 88 snowmelt, which remains in soil water towards the end of the growing season. Adaptation of the EcH2O-iso model provided an 89 opportunity to examine spatial patterns of frost depth throughout the catchment and its ecohydrological influence. Soil frost responded to both lower winter temperatures (increasing frost depths) and greater snowpack depth (decreasing frost depth). While 90 91 there was little influence on the overall timing of water movement at the catchment scale as stream water ages, the greatest influence 92 was observed within the ecohydrological partitioning, notably with the transpiration ages. Soil frost delays the onset of vegetation 93 growth and soil evaporation, resulting in older soil water from the previous autumn to sustain early-season transpiration rather than 94 younger snowmelt. With the implications of reduced numbers of cold days (Guttorp and Xu, 2011), and the dependence of vegetation growth on the summer temperatures (Schöne et al., 2004) in northern latitudes, this assessment of ecohydrological 95 96 partitioning is timely in understanding the effect of climatic change. 97

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