Response to the reviewers

We would like to express our gratitude towards the two anonymous referees for their constructive comments and for pointing out ambiguities and inconsistencies in the paper. We value very much their help in our effort toward a revised version of the manuscript. In the following, we write our point-by-point response in blue.

Referee 1:
We thank anonymous referee 1 for his/her comments.

The manuscript "Simulating hydrology with an isotopic land surface model in western Siberia" by Guglielmo et al. addresses a critical limitation in many land surface and hydrological model: the frequently inadequate partitioning of evaporative water fluxes due to evaporation and transpiration. Given the importance of a suitable representation of these processes not only as input into GCMs, the objective of this manuscript is to test in how far isotope data can help in meaningfully separating and constraining these processes, which comes timely and may in principle of interest to many in the community.

While the manuscript is well structured and clearly written, I do have some serious reservations about the relevance and validity of the results as I am far from convinced that the methods applied reflect the state-of-the-art in our understanding of how soils store and release water. Much of the model itself as well as the interpretation of the results are, at least it seems to me, based on the assumption that drainage and evaporative (i.e. evaporation and transpiration) water originate from the same pool of water. This is in stark contradiction to the growing experimental and modelling evidence on a range of spatial scales that this is not the case. In particular, a significant body of recent literature supports the hypothesis that water that is at least transiently stored in the soil matrix (and that thus is available for transpiration) is becoming older relative to the water being released by drainage the wetter the soil and the lower the soil moisture deficit. This is at this point thought to be the case as during dry conditions, high negative pore pressure "sucks" water into the smaller pores where it is rather tightly bound. As the system wets up, the suction reduces, less water can be stored in the small pores and thus remains in larger pore spaces where flow velocities are higher, contact times and contact surfaces with resident water are lower. Water entering the system under wet conditions will therefore experience less exchange ("mixing" or "dispersion") with resident water as it effectively starts to bypass the matrix through preferential flow paths (see recent experimental and modelling work by e.g. Brooks et al., 2010, Nature Geoscience; Botter et al., 2011; Hrachowitz et al., 2013, HESS; Evaristo et al., 2015, Nature; Benettin et al., 2015; WRR; Harman, 2015, WRR). The overly simplistic conceptualization of these transport processes in the model used in this study therefore makes me wonder, in how far the model processes do actually represent real-world processes.

-In ORCHIDEE-iso, the soil water isotope budget, although derived from a simple bucket model, is not treated as such. Soil water $\delta^{18}O$ vertical profiles are re-calculated at each time step, based on a multilayer isotope discretization (see text in supplementary material and scheme in Fig. S1). The isotope column is subject to soil evaporation at the surface layer only, to root extraction in the root zone, and to drainage at the bottom. Therefore it is not necessarily the same pool of water that feeds evaporation, root extraction, surface runoff and drainage. Moreover, surface runoff originates directly from precipitation, without any fractionation occurring.

We acknowledge lack of clarity in the text used to describe the mechanisms of water storage and release in the model, in particular for what concerns the water isotopic composition, e.g. in the description of the vertical discretization (e.g. in 9401.l8). Figure 2 is, moreover, very misleading, as it induces the reader to believe the isotopes follow the water discretization of the 2-layer bucket model used in the simplified representation of the hydrology in ORCHIDEE. Please, refer to Fig 2_new (below) and to Fig. S1. Furthermore, we think that the term 'diagnostic' as in 'diagnostic vertical discretisation' in the text is misleading and we will accordingly eliminate it.

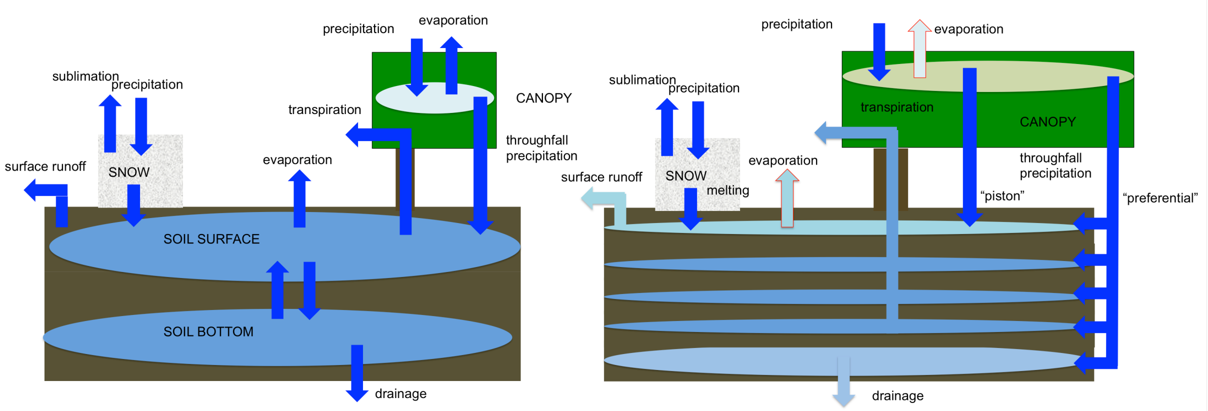

Fig. 2_new: Water budget and vertical discretization in the 2-layer hydrology in ORCHIDEE (left) and treatment of water isotopes (right; for a thorough description of the vertical discretization for isotopes, please refer to S1 and Fig. S.1). In spite of the crude vertical discretization of the 2-layer model (Choisnel et al. 1995), the hydrological processes are more realistically represented in the multi-layer representation used for isotopes modeling. The 2-layers water budget is not influenced by the treatment of the isotopes' composition that remains, in turn, coherent with the former. Fluxes of water and isotopic composition are calculated sequentially. Arrows with red borders (right) denote processes for which isotopic fractionation occurs.

In ORCHIDEE-iso, the degree of separation of the water pools, or "hydrologic connectivity", can be varied in the model by varying (1) the infiltration pathway (piston flow -following Darcy's law- or preferential pathway), (2) the diffusivity within the soil column, (3) the surface runoff/drainage proportion.
As we tested in this study (1), (2), but not (3), we fully acknowledge the fact that testing the surface runoff/drainage proportion would have added robustness to our approach. We will perform these tests for a revised version.

The processes behind pool segregation are not understood yet, nor are they at the moment exactly described in land surface models. To quote Bowen (2015): "The mechanisms that maintain the segregation of these pools of water as they move through the soil matrix remain unresolved, but understanding them is crucial for developing accurate models of soil-water partitioning."

Most land surface models designed for coupling within climate models implicitly represent the separation of different water pools through the temporal variability of water inputs, the vertical discretizations, and the different treatment between surface runoff and drainage. It is also the case for ORCHIDEE-iso (de Rosnay et al. 1998, Krinner et al. 2005). More sophisticated mechanisms for water pool separation are not implemented in such models, because such mechanisms are not yet well understood in nature (Bowen, 2015: "the relative roles of physical and temporal segregation remain unclear"). So ORCHIDEE-iso is far from being lagging behind from this point of view.

Following from that, and as the remaining analysis is largely based on a parameter sensitivity analysis of the model, I am not sure that the reported results/interpretation do have any significant physical meaning or if they merely illustrate the sensitivity of a “wrong” model. The authors themselves point out that the modelled isotopic profiles do not exhibit good match with the observed profiles. This is in particular true for Deuterium but also for the O-18 peaks at depth, which are attributed to seasonal effects.

The authors list a variety of (speculative) reasons for this mismatch, but go on as treating their model as a “valid” (sorry cannot think of a better word now) representation of reality. In general there is always a risk involved in virtual experiment approaches, where models are used to learn about processes, as is done here. Therefore, it is a widely acknowledged requirement for such approaches that the models used need to *at least* achieve a good fit with the observed data, so that they can be considered at least partially reasonable representations of reality. Only from such a starting point (as imperfect it is) further virtual experiments (e.g. analysis of which parameters and thus which processes control the response) can result in meaningful interpretations. From that perspective I am not convinced that the presented model fulfils these requirements and can be used to infer meaningful insights on real system behaviour.

-Our profiles are not matching the secondary peak in the depth for the stations showing it. We acknowledge that the text is not clear enough about the fact that as the worst mismatch with the observation is shown for station 2, we did not base any further analysis on this profile.

We will reformulate the text presenting the analysis eliminating ambiguities between actual evidence and speculative hypotheses.

The sensitivity analysis is performed to show which effect the different parameters have on the profiles. The result is that within the space of the parameters tested, the processes influencing the shape of the profiles, namely in first place the infiltration pathway, should be better investigated and represented, so we invoke further model testing and development, rather than draw conclusions about the system behavior.

Apart from that, minor and major points include:

(1) In general I found that much of the more recent literature in the general topic was ignored and it may be beneficial for the paper to consider the latest developments in a bit more detail (e.g. Brooks et al., 2010; Nature Geoscience; Sutanto et al., 2012, HESS; Hrachowitz et al., 2013; HESS; Jasechko et al., 2013, Nature; Klaus et al., 20913; HESS;

Coenders-Gerrits et al., 2014, Nature; Sutanto et al., 2014; HESS; Wang-Erlandsson et al., 2014, Earth Syst. Dyn.; Evaristo et al., 2015, Nature; Harman, 2015, WRR; Rinaldo et al., 2015; WRR)

-We will provide a better overview of the state-of-the-art modeling and observation landscape. We will make sure we integrate all these suggested references.

(2) P.9396, l.1: replace “confirm” by “test”

-OK

(3) P.9397, Eq.3: should the equation not read d-excess=deltaD-(8*delta18O+10) ??

-A typing mistake occurred upon submission. The equation will be rewritten in its correct form.

(4) P.9397,l.18-22: maybe link explicitly to fractionation here

-OK. The fractionation in ORCHIDEE will be moreover described in Supplementary Material.

(5) P.9398, l.10: precipitation is ALWAYS a flux (even if annual volumes are reported), i.e. needs to have the dimension L/T (or here specifically mm/yr)

-This will be corrected.

(6) P.9398, l.11: what is a short growing season? Please be more specific and give the months

- The sentence will be reformulated as: “…and a growing season of grasslands beginning in early June and ending in October.”

(7) P.9398, l.12/Fig.1: please indicate the exact positions of the stations with a symbol.

-We indicate the exact positions of the stations in Fig.1_new.

Figure 1_new. The territory of Labytnangi with the measurement sites indicated. Image from Google Earth, map data: Image ©2016 CNES/Astrium, Image ©2016 DigitalGlobe, Image Landsat, ©2016 Google.

(8) P.9399, l.5-14: I have never worked with vacuum distillation. I was wondering how much of the water stored in a soil sample can be extracted with that method? 100%? If it is less, one has to be careful about the interpretation of the isotopic signature: while more mobile water will be extracted, water bound more tightly (with a potentially different isotopic signature) will be extracted to a lesser degree. It will then be difficult to interpret which pool of water the sample represents.

-This is a mistake that occurred in the writing phase of the paper. The method to extract water from soil samples in the lab facilities at the University of Yekaterinburg was not vacuum distillation, but a methodology based on ‘squeezers’ (e.g. in de Groot 2008), to press out water from soil samples by using a press and some hand made facilities. The principle is to press out water from a soil sample to avoid phase transition and, thus, isotope fractionation. We expect the amount of water extracted from the soil samples to be within 95-100%, closer to 100%.

The sentence “The water was then extracted from the soil samples by vacuum distillation" will be replaced by another, along the lines of "The water was then extracted from the soil samples by a conventional method using ‘squeezers’ in order to press out of water from the soil cores. The extracted water samples were filtered and then analyzed with a laser PICARRO instrument to determine the $\delta^{18}O$ and δD".

(9) P.9400, l.9ff: more detail about the model is necessary in order to understand what was done and how. For the convenience of the reader I would also suggest to provide the relevant set of equations in the supplementary material, even if it was already published elsewhere before.

- In Supplementary Material we provide the equations used for vertical discretization for isotopes and for fractionation processes. The manuscript text will be revised to avoid redundancies and will contain references to this material where opportune.

(10) P.9400. l.15: the parameters used in the model are provided without any further justification and seem rather arbitrary. In particular, where do the 300mm water holding capacity come from? What is the reasoning for using the same value for all 4 sites? As I understand (and as it is used in most hydrological models), the water holding capacity is the storage capacity in the root zone between field capacity and wilting point. Below the root zone, the water content of the unsaturated zone will be on average at around field capacity (no water can be extracted by roots!). In the root zone, the storage capacity will be controlled by vegetation (i.e. the water volume accessible to roots; Gao et al., 2014; GRL) and soils and will thus vary from site to site.

- In the ORCHIDEE version used in this study, the holding capacity is variable spatially with soil depth. Soil depth can vary from 2m to 4m. The default value for the holding capacity is indeed 300mm.

Similarly, a static runoff partitioning (95% drainage, 5% fast runoff) cannot be seen as a plausible representation of reality, as it goes against any type of experimental evidence and the concept of hydrological connectivity. In a nutshell, this is a experimentally well established positive feedback process: the wetter a system, the higher its connectivity, the higher the proportion of fast/preferential/surface runoff. It remains also unclear how isotopic fractionation due to soil evaporation was implemented. More detail is needed here to assess the model.

- We acknowledge this remark. The sensitivity of the system to this proportion will be checked in further sensitivity tests.

We understand that experimental evidence suggests that the proportion of surface runoff over total runoff should increase as the soil moisture increases. However, this effect cannot be taken into account in the Choisnel hydrological scheme used in this study, because runoff occurs only when soil is saturated, i.e. the runoff occurs always for the same value of soil moisture. However, we can mimic this effect by considering higher proportions of surface runoff over total runoff for stations associated by higher soil moisture. To explore this effect, we are performing additional sensitivity tests to the surface runoff/drainage proportion.

A description of how isotopic fractionation due to soil evaporation was implemented will be added in the Supplementary Material.

(11) P.9401,l.3ff: this section remains rather vague. How was the isotopic composition in each layer estimated? By vertically and routing each individual input signal and summing all partial signals in each layer up at each time step?

-See scheme in the new figure S.2.

(12) P.9402, l.2: what is gtau?

-Typo: what is meant here is τ.

(13) P.9404, l.14ff: for which time period was the model run? Which parameters other than the ones discussed had to be selected ("tuning") and how was this done?

-The model was spun up for five years and then run for the year 2012. The parameters tuned for this study were the three indicated in table 2, namely the infiltration pathway, the product $\theta_l\tau$, and the extinction coefficient. The set of values for each parameter was indicated in Fig. 5-7. The model was run once for each combination of values. Results where compared to the experimental profiles and values leading to 'best fits' selected for the evaluation.

How meaningful is it to run a model on a 6-hourly basis(!), if the available isotopic input data have a temporal resolution of one month(!)???

- We will rewrite the model description to clarify that ORCHIDEE was run at 30min time step.

The local forcing, available each 6h, has been interpolated at 30min time resolution following the methodology developed by Viovy et al. (1997). It is crucial to represent the hourly, diel and synoptic variability of the meteorological forcing, as covariations between different forcing variables are strong at these time scales.

Ideally, isotopic forcing should also be available at these time scales (Henderson-Sellers 2006). Variations of the isotopic composition of precipitation and water vapor in Siberia at these time scales can be significant (Gryazin et al. 2014). It is possible, for example, that most intense precipitation events are associated simultaneously with more depleted values and more efficient surface runoff, so that the water that infiltrates the soil is systematically more enriched than the average precipitation. However, isotopic forcing is not available at this time scale. Sites where hourly isotopic observations of precipitation and water vapor and isotopic observations of soil water are available are extremely scarce. We could use isotopic GCM outputs, but our confidence in the capacity of GCMs to simulate the short-term, local variability in isotopic composition of precipitation is limited. Therefore, we decided, as a first study, to use monthly isotopic forcing.

We will add a few sentences in the text to express this reasoning and its consequences. Based on high-frequency data from Gryazin et al. 2014, we will calculate an upper bound for the systematic bias that could results from neglecting the covariation between precipitation composition and precipitation rate.

(14) P.9405, l.24-26: speculative, can be removed if no further evidence is presented.

-This sentence will be removed.

(15) P.9406, l.6: this is vertical *dispersion*, really, because much of the movement is advective

We will replace “vertical diffusion” with “dispersion” everywhere.

(16) P.9406, l.14-24: possible, but again rather speculative in the absence of data supporting this.

-This text portion will be reformulated. For clarification: the higher permeability of station 2 is related here to the coarser soil texture and to the absence of a top peat horizon, able to accumulate significant amounts of water (Valdayskikh et al. 2013). As for the existence of a seasonal signal, we base our inference on the composition of precipitation data (Gryazin et al. 2014), as winter observations of isotopes in soil water are not available for the Labytnangi territory.

(17) P.9408, l.28: no, the entire conceptualization of how water is stored and released is over simplified (See above).

-This sentence will be reformulated. Among others, “vertical transport processes will be replaced by “vertical dispersion”.

(18) P.9409,l.1.13: difficult to assess as no details are given of how e.g. fractionation is handled in the model.

-We add details on fractionation in Supplementary Material.

(19) P.9409, l.14: with a hindsight it may have been more instructive to take isotope profiles at different points throughout the year and test if the model can reproduce the temporal changes in isotopic signatures integrated over the entire respective soil profiles.

-Yes, we agree. Unfortunately in Labytnangi, as in other boreal regions, only measurements taken in summer months are available.

(20) P.9414: quite frankly, I have not quite understood the reasoning behind this part of the analysis and I can therefore not comment on its feasibility.

- We acknowledge lack of clarity here, both in text and figure caption. We will reformulate the text in both, in order to better introduce and describe methodology and results.

Referee 2:
We thank anonymous referee 2 for his/her comments.

The paper, however, is inconclusive about the main question raised in the title, namely, what can we learn from water isotopes.

-We acknowledge the fact that what our title promises something going beyond the quantity and quality of the information we deliver, and are accordingly changing the title to: “Simulating isotopic composition of water in western Siberia with a land surface model”.
We believe nevertheless that this paper still shows, to some limited extent, that water isotopes help understanding processes in land surface models.

The reasons, in my opinion, have to do with 2 aspects:

1. The large uncertainty in the data and boundary conditions.

With respect to the data, the vertical soil profiles at the 4 stations were measured in August. They therefore represent one point in time, and they do not provide indications about the existence of seasonal dynamics.

-One limitation of this study is, indeed, that the measurement campaign could not be extended in time, due to environmental constraints. We do, however, have the seasonal dynamics of the forcing, based on observed isotopic composition of precipitation at nearby stations and on GCM outputs.

The isotope input data are available at monthly time scales, with contrasts with the model time step of 6 hours. This makes wonder whether, given such coarse input data, the 6 hours simulations may be considered representative of isotope dynamics at fine time resolution.

-The model time step (i.e. the integration step) is of 30 minutes (pages 9400-9402). ORCHIDEE needs meteorological forcing at high frequency (6 hours). The output frequency is monthly.

We will rewrite the model description to clarify that the ORCHIDEE model is run at 30mn time step.

Moreover, the input data are available at stations far apart the experiment 360, 970 and 980 km respectively. The Authors say that they interpolated between these values. But this does not save them from a potentially exceedingly large input uncertainty.

-From the manuscript text: "The values at the three different forcing stations were further spatially interpolated to the study area assuming the same spatial patterns as those obtained by an isotopic simulation of the isotope-enabled atmospheric GCM LMDZ-iso".

For clarification purposes we will provide in detail the methodology (Risi 2009) used to calculate the isotopic forcing in Supplementary Material.

We acknowledge that this method has several sources of uncertainties:

1) uncertainties with erroneous spatial structures in LMDZ so that model-data differences vary from one station to the next;

2) uncertainties associated with spatial structures finer that the GCM grid cells (<250km) that are not reproduced by LMDZ;

3) uncertainties in the isotope-altitude simulated by LMDZ;

4) uncertainties in the precipitation-vapor composition difference.

Sources of uncertainties 1 and 4 are relatively limited given the good performance of LMDZ for these aspects, as evaluated by Gryazin et al. 2014 and Pommier et al. 2014.

This information will be integrated in the brief discussion on uncertainty in the description of the isotopic forcing, complementing the information on the temporal frequency/variability of the same (see above).

The model is applied point wise. As far as I understood, the exchange is assumed to occur only with the atmosphere. What about groundwater flow, lateral flow, and all other potential impact about other inputs? These are not mentioned and discussed.

-ORCHIDEE-iso does not take into account groundwater and lateral flow (we believe this does not greatly affects simulations in the region of Labytnangi whose terrain is flat and underlain by permafrost). However, very few large-scale land surface models do (stated e.g. in Zhao and Li 2015, Choi et al. 2013).

We will improve the overview on state-of-the-art models and datasets in the introduction.

2. The absence of comparisons with alternative isotope models.

With respect to the second point, the Authors provide a certain process description, which is basically assumed. In order to convince the readers that such description is appropriate, the Authors should have at least compared it with some alternative descriptions.

A more conclusive study requires changing the location to a place where more data are available and more extensive analysis can be carried out.

-We acknowledge that our introduction and model description lack a proper overview on the isotope modeling landscape in term of processes. We are listing here some references we will appropriately integrate in the text, alongside the ones already cited:

Isotopic Land Surface Models : Cuntz et al. 2003, Haese et al. 2013, Yoshimura et al. 2006, Riley et al. 2002, Aleinov and Schmidt 2006.

More detailed models, not for coupling with GCMs are cited (Melayah et al. 1996, Braud et al. 2005) in different parts of the text.
Model inter-comparison project: iPIPLS (Henderson-Sellers et al. 2006), which involved old versions of land surface models.

ORCHIDEE-iso has been extensively tested at different locations, representative of different climates in a previous study (Risi 2009).

It would be indeed desirable to have temporal series of data; however full seasonal cycles in soils are available only for a few sites in the world, even fewer for boreal regions. Moreover, for these latter regions only measurements taken in summer months are available.

Moreover, it would be necessary to do some “hypothesis testing” with the proposed model developments. This analysis would help to support statements such as “The model performed relatively well in simulating some features of the ^{18}O soil profiles”.

Relative to what?

-Yes, we agree. This very sentence will be reformulated.

Other points:

The paper is not clearly written. For example, in the abstract: “In this paper, we investigate the usefulness of water stable isotopes in land surface models studying land surface processes. To achieve this, we implemented. . .”. What does “this” refer to?

-These sentences will be reformulated along the lines of: “In this paper, with the aim of investigating the usefulness of water stable isotopes in land surface models studying land surface processes, we implemented. . .”.

There are many examples like this in the paper, such as the following one in the introduction. “The fact that the isotopic composition of water is affected by phase changes makes it a reliable tracer”. What does “it” refer to?

-We will reformulate this sentence as: “The isotopic composition of water is affected by phase changes and can therefore be used as a tracer for the hydrological cycle” and try to clarify other ambiguous points.

A native English speaker will moreover proofread the whole manuscript.

Equation 3 is wrong, or at least it does not follow from Equation 2.

-This is a typing mistake that occurred upon submission. The equation will be corrected.

Page 9397: “Moreover, at least two hydrological regimes (swamp, alluvial plain) are identifiable”. Is alluvial plain an hydrological regime?

-The sentence will be eliminated.

References:

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Supplementary Material

S.1 Vertical discretization of the isotopic composition in ORCHIDEE-iso

The isotopic composition is discretized in in ORCHIDEE-iso (Risi 2009) in layers that are progressively filled with the available soil moisture. The first layer has thickness

$$L = \sqrt{K_D \cdot dt} \qquad (S.1)$$

where K_D is the diffusivity of isotopes in soil water. K_D has been calculated according to Braud et al. (2005), neglecting the dispersion term, as:

$$K_D = D_m \cdot \theta_l \cdot \tau \qquad (S.2)$$

where D_m [m^2/s] is the molecular self-diffusivity of water, θ_l [unitless] is the volumetric content of liquid water (function of the depth, constant in time) and t [unitless] is the soil tortuosity. Independently of the temperature, the value attributed to D_m is 2.5·10−9 m^2/s for all isotopes considered (Harris and Woolf 1980). Braud et al. (2005) suggest for the product $\theta_l \cdot \tau$ the value 0.1. Different values for this parameter are tested in the paper. The value of L corresponding to the time step used in this study, 30 min, is then of about 0.7 mm. This is consistent with a value of 0.67 for τ (e.g. Braud et al. 2005) and with an average of about 15% for θ_l. Vapor diffusion in soil and possible associated fractionation are not considered (Melayah et al. 1996).

Further layers have fixed thickness $l = L \cdot r$. Parameter r has a default value of 30, corresponding to l =21 mm. The bottom layer has a thickness varying between 1 and 2 l so that the total soil equivalent water height in the whole soil columns is equal to the sum of the water heights of the single layers.

Maximum equivalent water height in 2-layers ORCHIDEE (Choisnel et al. 1995) is 300mm in a 2 meters deep soil. Soil depth is a prescribed and spatially variable parameter. If the soil is saturated, n=16 layers are present by default in ORCHIDEE-iso. Whenever water is added or subtracted to the water budget, the discretization is recalculated keeping the mass of isotopes and the isotopic profile unchanged.

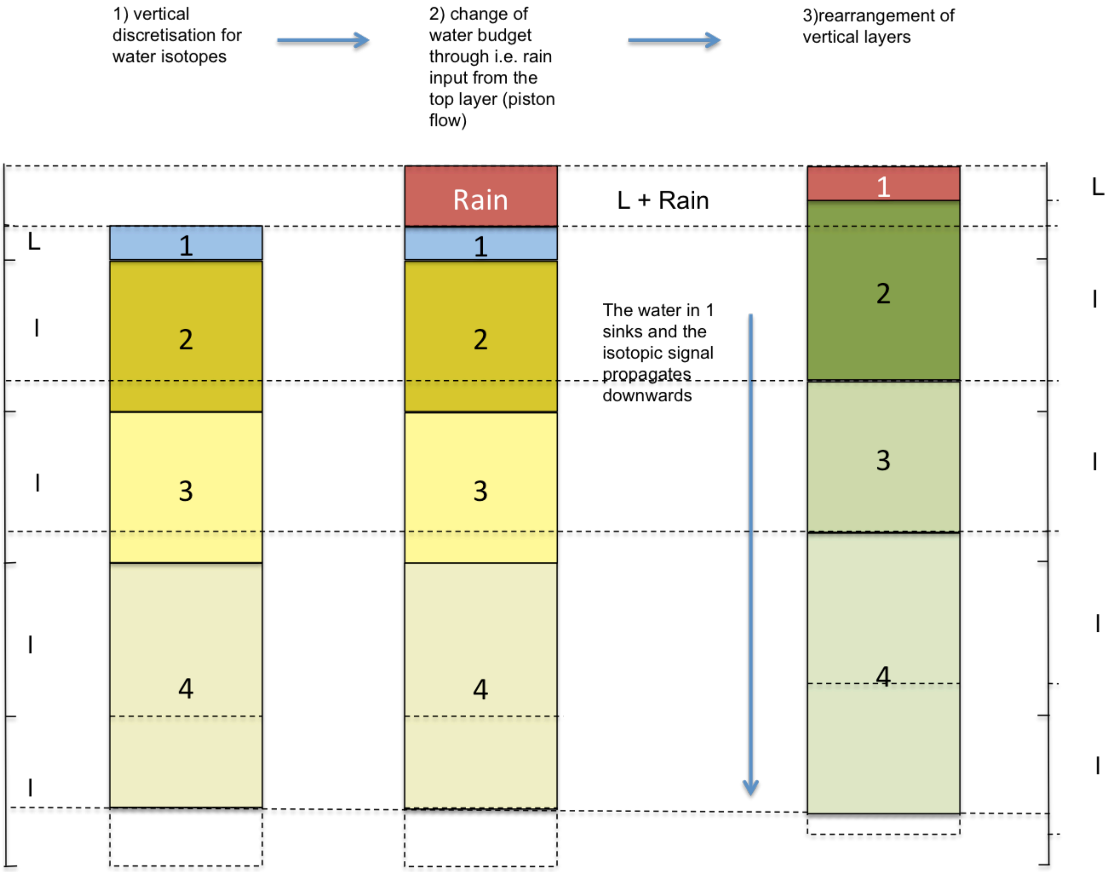

Fig. S.1 vertical discretization (1), change of the water budget (2), subsequent rearrangement of the vertical layers (3). For this sketch r = 4.5 => l=4.5 L.

S.2.Evaporation and transpiration

Bare soil evaporation occurs in ORCHIDEE from the first layer; should the equivalent height of the evaporated water exceed the one of such layer then water is also extracted from the layer(s) underneath.

Water subject to transpiration comes in ORCHIDEE from layers below the first one (de Rosnay 1999). An exponential root extraction profile, in accordance with the way water stress is calculated in the Choisnel model (Choisnel et al. 1995) is assumed in the model: the fraction of water subject to transpiration in each layer i > 1, delimited above by z_{i-1} and below by z_i, is, with respect to the total transpiration:

$$\frac{T_i}{\sum_{i=1}^{n} T_i} = \frac{\int_{z_{i-1}}^{z_i} e^{-h \cdot z}}{\int_{z_1}^{z_n} e^{-h \cdot z}} \qquad (S.3)$$

h is in ORCHIDEE a constant and depends on the vegetation type.

S.2.1 Evaporation and fractionation

Input fluxes (precipitation, dew, snow thawing) are added to the soil reservoir during the previous time-step. We neglect here water vapor. Knowing the evaporation flux E, we calculate the isotopic evaporative flux $x_{E.}$. Following Craig and Gordon (1965), the isotopic ratio of the evaporation flux at the soil/atmosphere interface $R_E(t) = \frac{x_E}{E}(t)$ is provided by the equation:

$$R_E(t) = \frac{R_l(t) - \alpha_{eq} \cdot h \cdot R_v(t)}{\alpha_K \cdot \alpha_{eq} \cdot (1-h)} \qquad (S.4)$$

where $R_l(t)$ is the isotopic ratio in soil (liquid) water subject to evaporation, $R_v(t)$ and h are isotopic ratio and relative humidity of the atmosphere above the soil surface, respectively, α_{eq} and α_K are equilibrium and kinetic fractionation coefficients, respectively.

Considering that the vapor reservoir in the boundary layer is much bigger as compared to the evaporation, we treat $R_v(t)$ as a constant and equal to the initial $R_v(0)$, i.e. we assume variations of R_v during the evaporation process to be non-significant (first order approximation for the vapor). We follow, on the other hand, the evolution of R_l during the evaporation process:

$$dR_l = \frac{dm_l}{m_l} \cdot \left(\frac{x_l}{dm_l} - R_l\right) = \frac{dm_l}{m_l} \cdot (R_E - R_l) \qquad (S.5)$$

where ml refers to the mass of water and xl is the isotopic equivalent of m_l .

Replacing R_E with its expression from Craig and Gordon (1965):

$$R_E = \frac{1}{\alpha_k} \cdot \frac{\frac{R_l}{\alpha_{eq}} - h \cdot R_v}{1-h} \qquad (S.6)$$

we obtain:

$$dR_l = \beta \cdot (R_l - \gamma \cdot R_v) \cdot \frac{dm_l}{m_l} \qquad (S.7)$$

β and γ are coefficients function of the relative humidity as:

$$\beta = \frac{1 - \alpha_{eq} \cdot \alpha_K \cdot (1-h)}{\alpha_{eq} \cdot \alpha_K \cdot (1-h)} \qquad (S.8)$$

$$\gamma = \frac{\alpha_{eq} \cdot h}{1 - \alpha_{eq} \cdot \alpha_k \cdot (1-h)} \quad \text{(S.9)}$$

Integration of equation S.7 yields (Stewart, 1975):

$$R_l = R_l(0) \cdot f^{\beta} + \gamma \cdot R_v(0) \cdot \left(1 - f^{\beta}\right) \quad \text{(S.10)}$$

where $R_l(0)$, $R_v(0)$refer to the beginning of the evaporation processes, $f = \frac{m_l}{m_l(0)}$, with $m_l(0)$ initial soil water amount and m_l residual amount.

In the limit case $h = 0$ (dry air), R_l follows an inverse Rayleigh distillation:

$$R_l = R_l(0) \cdot f^{\beta}. \quad \text{(S.11)}$$

For $h = 1$ (saturated air), the droplets establish equilibrium with the surrounding vapor:

$$R_l \rightarrow \alpha_{eq} \cdot R_v \quad \text{(S.12)}$$

The average evaporation over the evaporation process, R_E, can be calculated by a mass conservation equation: the isotopes in the initial liquid are redistributed among final liquid and vapor phase:

$$m_{l(0)} \cdot R_l(0) = m_l \cdot R_l + (m_l(0) - m_l) \cdot R_E. \quad \text{(S.13)}$$

Replacing R_l with its expression from the Stewart equation S.10 above:

$$R_E = \frac{R_l(0) \cdot (1 - f^{\beta+1}) - \gamma \cdot R_v \cdot f \cdot (1 - f^{\beta})}{1 - f} \quad \text{(S.14)}$$

Other approaches as listed in Risi (2009): due to a very short dt (less than one minute) and to a very fine vertical discretization (< 1mm), Melayah et al. (1996) use a zero-order approximation of Craig and Gordon formulation. For this current study, with a dt of 30 minutes, we cannot neglect time variations of $R_l(t)$. The calculations used for this study are coherent with the formulation of drops re-evaporation in the convection scheme adopted in LMDZ (Bony et al. 2008), except for the 1st order approximation for water vapor.

For h=1, equation S.9 is not applicable (Stewart 1975). One assumes then that the soil is subject to a partial re-equilibration, via diffusive exchanges, with the overlying vapor.

The composition of the isotopic evaporation x_e, is calculated via mass budget, assuming that the upper soil layer (of height L) reaches isotopic equilibrium with an amount m_v of water vapor above:

$$x_E = \frac{L \cdot m_v \cdot (R_{l0} - \alpha_{eq} \cdot R_{v0}) + E \cdot \Delta t \cdot (L \cdot R_{l0} + \alpha_{eq} \cdot R_{v0} \cdot m_v)}{m_v + E \cdot \Delta t + (L - E \cdot \Delta t) \cdot \alpha_{eq}} \qquad \text{(S.15)}$$

S.3 Methodology for the calculation of the isotopic forcing

For each (i) on n stations and for each month, the enrichment in precipitation $\delta_{forcing}$ is calculated as follows:

$$\delta_{forcing} = \delta_{LMDZc} + \sum_{i=1}^{n} \left(r(i) \cdot \left(\delta_{obs}(i) - \delta_{lmdz}(i) \right) \right) \qquad \text{(S.16)}$$

δ_{LMDZc} expresses here the enrichment calculated by the isotopic atmospheric GCM LMDZ adjusted to the altitude z_{obs} of observation and simulation locations:

$$\delta_{LMDZc} = \delta_{LMDZ} + a \cdot (z_{obs} - z_{lmdz}) \qquad \text{(S.17)}$$

a is here the slope of the δ_{LMDZ} curve as a function of the altitude.

The term r(i) is calculated as follows:

$$r(i) = \frac{1}{d(i)} \cdot \sum_{i=1}^{n} \frac{1}{d(i)} \qquad \text{(S.18)}$$

where d(i) indicates the distance between the ORCHIDEE site and the observation sites.

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