

Response to Reviewer 2

We thank Reviewer 2 for the comments on the different aspects of the manuscript. We answer them below (in blue) and will make changes accordingly in the revised manuscript.

- **Major comments**

As I said in the introduction, one major problem of the complex ESMs is the computing time. From this perspective, iLOVECLIM is very useful for paleoclimate simulations. The drawback of this model is the rough spatial and time (?) resolutions. I think this aspect of iLOVECLIM should be more emphasized in the introduction. Still for the introduction, this is in my knowledge the first time that ^{17}O -excess is modeled in a coupled atmosphere-ocean model. Until now, only the atmospheric model LMDZ-iso was able to simulate the H_2^{17}O isotopologue (Risi et al., 2013). This should be clearly stated in the abstract and the introduction.

Thank you for this comment. We added a new paragraph in the introduction to synthesize previous work the work on isotope modelling with the climate models: *“Since the initial works of Joussaume et al. (1984) and Jouzel et al. (1987), much progress has been done in atmospheric general circulation models (AGCMs) (e.g. Hoffmann et al., 1998; Noone and Simmonds, 2002; Mathieu et al., 2002, Risi et al., 2010; Werner et al., 2011) that can simulate accurately the $\delta^{18}\text{O}$ of precipitation. The subsequent development of water isotopes modules in oceanic general circulation models (OGCMs) (Schmidt, 1998; Delaygue et al., 2000; Xu et al., 2012) opens the possibility for coupled simulations of present and past climates, conserving water isotopes through the hydrosphere (Schmidt et al., 2007; Zhou et al., 2008; Tindall et al., 2009; Werner et al., 2016; Cauquoin et al., 2019). In general, General Circulation Models (GCMs) have been used exclusively to simulate separately water isotopes in the atmospheric and oceanic components. Given the computing resources needed to run coupled climate models, applying intermediate complexity coupled climate models with water isotopes like iLOVECLIM to long-term palaeoclimate perspectives still appears quite suitable (e.g. Caley et al., 2014). It could allow to improve our understanding of the relationship between water isotopologues, second-order parameter (like d-excess) and climate over a broad range of simulated climate changes”.*

With respect to the ^{17}O -excess we also added the following text in the introduction to highlight that very few model simulate this proxy: *“Modelling the ^{17}O -excess is still very challenging since it depends on complex processes that have to be properly reproduced in the climate models. To date, only the LMDZ4 model has included the ^{17}O -excess (Risi et al., 2013). However, even if the processes that control the ^{17}O -excess are more complex than those controlling the d-excess, the combination of the d-excess, ^{17}O -excess and ^{18}O could bring new information on the understanding of past changes in local temperature, moisture origin and conditions at the moisture source”.*

We also clearly stated in the abstract that we present modelled ^{17}O -excess results. This now reads: *“Following previous developments of $\delta^{18}\text{O}$ in the coupled climate model of intermediate complexity iLOVECLIM, we present here the implementation of the $\delta^2\text{H}$ and $\delta^{17}\text{O}$ water isotopes in the different components of this model, and calculate the d-excess. We also present results of modelled ^{17}O -excess in the atmosphere and ocean, that was currently only available in the LMDZ4 model The modelled ^{17}O -excess presents a too important dispersion of the*

values in comparison to the observations and is not correctly reproduced in the model mainly because of the complex processes involved in the ^{17}O -excess isotopic value”.

Still for the introduction, for which kind of paleoclimate applications ^{17}O -excess is useful? More generally, a paragraph of the introduction should be a review of the paleoclimate studies (recent if possible) using of d-excess or ^{17}O -excess. For d-excess, such recent studies exist like Landais et al. (2021). For ^{17}O -excess, I do not see to be honest as the measurements can be challenging. However, the author should try to explain how the ^{17}O -excess can be used, not only by just saying that it is proxy of the relative humidity over the ocean. This kind of context information is necessary because simulating d-excess and ^{17}O -excess is very challenging.

Thank you for pointing out this aspect. In the revised version of the manuscript, we developed the ^{17}O -excess paragraph in the introduction to provide some context on this proxy. The following text has been added in the introduction: *“The ^{17}O -excess is commonly used in ice core based paleoclimate studies to give information on the relative humidity over the ocean (e.g. Landais et al., 2008, 2018; Risi et al., 2010; Steig et al., 2021). ^{17}O -excess is controlled by kinetic fractionation during evaporation, and similarly to d-excess, very sensitive to empirical parameter determining the supersaturation in polar clouds (Winkler et al., 2012; Landais et al., 2012). Since influences of temperature or condensation altitude on ^{17}O -excess are expected to be insignificant in contrast to d-excess, measurements of ^{17}O -excess have an added value with respect to d-excess and can be used to disentangle the parameters (temperature, relative humidity) that affect the water isotopic composition. For example, Risi et al. (2010) shown that the different behaviors of d-excess and ^{17}O -excess in polar regions could be related to fractionation processes along the distillation pathway from the evaporative source to polar region that affect more the d-excess than the ^{17}O -excess, that record more the signal from low latitudes during surface evaporation. Modelling the ^{17}O -excess is still very challenging since it depends on complex processes that have to be properly reproduced in the climate models. To date, only the LMDZ4 model has included the ^{17}O -excess (Risi et al., 2013). However, even if the processes that control the ^{17}O -excess are more complex than those controlling the d-excess, the combination of the d-excess, ^{17}O -excess and ^{18}O could bring new information on the understanding of past changes in local temperature, moisture origin and conditions at the moisture source”.*

I expect to use this kind of models for diverse paleoclimate applications. But which ones are really possible with a reasonable confidence? Before really reading the paper, I thought it would have been great to not only simulate pre-industrial conditions but also another climate period further in the past. As it is not the case, I recommend to the authors to do a deeper evaluation of their simulation against present-day observations with more skill metrics like r^2 and root mean square errors, and a comparison of these metrics with the ones from other general circulation models (GCMs) when available. Moreover, the authors should show more clearly if the well-known isotope continental effect and the amount effect are well represented in iLOVECLIM, in comparison to observations and other isotope enabled GCMs (like they did for the latitudinal effect). Last but not least, the disagreement between model results and observations is explained by uncertainties in the latter several times in the manuscript (e.g., l. 264-265, 289-291, 272-273, 310, 320-321, 443-445). I think these are not very honest statements. Instead, I would formulate a more quantitative model-data comparison, which would help the readers to know for which paleoclimate applications and isotope effects

iLOVECLIM can be used. In this regard, the figures 4, 5, 6 and maybe 7 need to be changed or adapted.

Thank you for this comment. As also suggested by the reviewer 1 we added a new figure to summarize some skill metrics for our model results, for existing water isotopes-enabled models and for the observations. We also detailed the different continental, amount and temperature effects in our model by investigating them individually. We then compared them to existing models like LMDZ4 and ECHAM5-wiso. Please see response to the first reviewer in Section 1.1 for this aspect.

In this paper we only investigated the capacity of our model to reproduce the hydrogen isotopic composition, d-excess and ^{17}O -excess for present day, as it is a development paper. The simulation of the isotopic composition under another past climate period is not within the scope of this paper. But this opens new possibilities to perform long-term transient simulations with a model equipped with the isotopes since iLOVECLIM has the possibility to run simulations over several thousands of years within several weeks/months. For example, paper like Caley et al. (2014) already investigated past changes in the modelled oxygen isotopic composition during a glacial-interglacial cycle. We added a sentence in the manuscript to emphasize this aspect: *"Given the computing resources needed to run coupled climate models, applying intermediate complexity coupled climate models with water isotopes such as iLOVECLIM to future long-term palaeoclimate perspectives appear very promising. Paleoclimate simulations during the Holocene, Last Glacial Maximum or transient glacial/interglacial periods are the next logical step to compare model results against past isotopic composition records"*.

As already reported by the first reviewer, the fractionation for evapotranspiration is not supposed to be at equilibrium. Or there is no fractionation, like in MPI-ESM-wiso, or a fractionation using a bulk formula is used for the bare soil evaporation (i.e., kinetic, see the equation 6 from Haese et al., 2013). The simplest way is to perform another simulation without such fractionation in order to see the impact of your equation 10 and hopefully to improve the modeled results. Just an extension of a couple of hundred simulations should be enough, I guess.

Thanks for the remark and discussion of these processes. The text that is referred to was built from Roche (2013). A careful examination of the model code as used in the simulation presented in this study assumes no fractionation during all land-related evaporation processes, contrary to what was stated in the previous version of the manuscript. We removed Equation 10 and corrected the text accordingly: *"If re-evaporation occurs on land, it is assumed to be at equilibrium (without fractionation)"*.

Before reading in detail the paper, I have been astonished by the very high and low values of ^{17}O -excess, as well as their variations from one grid cell to another, in Figure 1. This is especially the case in Antarctica. As these are averages of several years, I guess these jumps are even worse from one year to another or at monthly scale. Honestly, I am worried by these huge variations. It is completely fine to not be able to represent very well the ^{17}O -excess in such models because it is an extremely hard task. If the authors cannot fix this issue, I would expect honest suppositions on the causes of the failure of iLOVECLIM in simulating ^{17}O -excess, instead of pseudo-explanations related to the uncertainties of the observations only. In addition, I suggest deleting all references and plots related to $\delta^{17}\text{O}$. $\delta^{17}\text{O}$ is not really used

in the literature and does not bring any new information compared to $\delta^2\text{H}$ (the spatial characteristics are similar for example). The important proxy here is ^{17}O -excess.

We agree and removed the $\delta^{17}\text{O}$ results (spatial distribution and model-data comparison) from the main text. Instead, we added an Appendix A for the $\delta^{17}\text{O}$ to show in a first figure the spatial distribution of the isotopic composition in the atmosphere and ocean and the model results against the observations in a second figure.

Based on the Taylor diagram and the model-data comparison, we observe for the ^{17}O -excess a low correlation coefficient for iLOVECLIM and a low negative correlation coefficient for LMDZ4 with respect to observations. The standard deviation and root mean square error is better for LMDZ4 than for iLOVECLIM (Fig. 1c), suggesting that our model does not correctly reproduce the ^{17}O -excess and has a too important dispersion of the values, even if the trend is correct. We now clearly state that iLOVECLIM does not correctly reproduce the ^{17}O -excess values and suggest that this is mainly because of the complex processes involved in this isotopic composition and because of difficulties in modelling the isotopic composition for area with very low humidity content (especially for Antarctic values). In comparison, LMDZ4 shows indeed much smoother variations and less dispersion than iLOVECLIM but presents a general trend that is the opposite to the one observed in the measurements suggesting that both models do not perfectly reproduce the ^{17}O -excess, but probably for different reason.

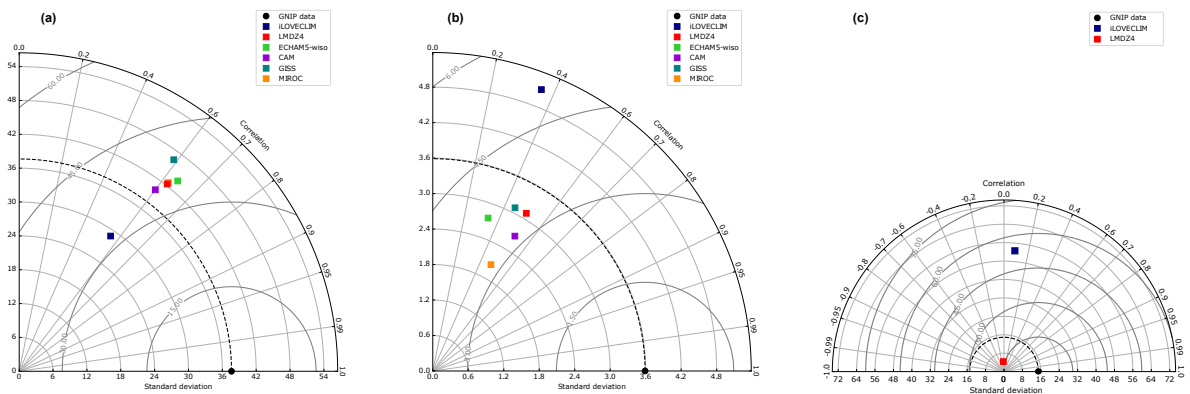


Figure 1: Taylor diagram representing (a) $\delta^2\text{H}_{\text{precipitation}}$, (b) d -excess and (c) ^{17}O -excess values for different climate models (iLOVECLIM, LMDZ4, ECHAM5-wiso, CAM, GISS and MIROC) without Antarctic values. The simulated values are plotted against the observations. The dotted curved line indicates the reference line (standard deviation of the observation) and the bold grey contours represent RMSE values.

Based on the new figures to evaluate the model metrics like model-observation correlation or RMSE, we now properly state in the revised manuscript that the ^{17}O -excess is not correctly reproduced in iLOVECLIM.

- **Line by line comments**

Title: I would change the title a little bit because the novelty here is to model $^1\text{H}^2\text{H}^{16}\text{O}$ and H_2^{17}O , not the ^{18}O . Moreover, iLOVECLIM models the isotopologues (i.e., molecules), not the atoms of hydrogen and oxygen.

We changed the title to “*Modelling water isotopologues ($^1\text{H}^2\text{H}^{16}\text{O}$, $^1\text{H}_2^{17}\text{O}$) in the coupled numerical climate model iLOVECLIM (version 1.1.5)*” to take into account this suggestion.

I. 14-15: is the simulation really under preindustrial conditions as the orbital year considered is 1950 and not 1850?

The insolation is taken from the year 1950 but the other boundary conditions are taken from the preindustrial.

I. 24: “Stable water isotopologues (H_2^{16}O , H_2^{18}O , $^1\text{H}^2\text{H}^{16}\text{O}$, H_2^{17}O), expressed hereafter in the usual d notation with respect to V-SMOW scale (Dansgaard, 1964), are important...”

Done.

I. 29: The term “however” sounds strange here.

We removed this term.

I. 53: not so new method.

We replaced “A new method” by “Another method”.

I. 61: same as above, the studies are not so recent. So, remove the term “More recently”.

Done.

I. 65: A paragraph could be written about the use of d-excess and ^{17}O -excess for paleoclimate studies. See major comment.

Done.

I. 99-100: the authors say they present the equations for deuterium only, but then the equations of ^{17}O are shown latter in the manuscript (equations 7 and 9). I would say instead that you introduce the equations for the heavy/light isotope ratios.

We modified the sentence accordingly.

Equation 4 is from Craig and Gorgon (1965).

We changed the reference in the text.

Section 2.3: please add the time steps of the atmosphere and ocean modules. Also, do all the results come from the 100-years simulation starting from the 5000-year spin-up simulation?

The atmospheric module has a timestep of 6 hours and the oceanic module has a daily timestep. We added these timesteps in the respective Sections 2.1 and 2.2 for the atmosphere and the ocean.

The 100 years simulation starting from the 5,000 years spin-up has been parametrized to display monthly outputs. So, it is only used to investigate the seasonal variations of the precipitation and isotopic composition in Section 3.1.4. The 5,000 years simulation has annual outputs only and is used for the rest of the manuscript. We specified in Section 2.3 that the 100 years simulation is only used to investigate the seasonal variations.

Section 2.4: I would also mention the results from other isotope enabled GCMs here or in a new subsection just after. In the former case, please rename the section appropriately.

We renamed the Section 2.4 into Observational data and water isotopes enabled GCMs. This section presents all the datasets used in the manuscript to compare with the model results. We also added a new paragraph to mention the other isotopes-enabled GCMs used in this manuscript that reads: “To evaluate our model results against water isotopes-enabled GCMs, we used several model outputs: ECHAM5-wiso (Steiger et al., 2018), GISS (Schmidt et al., 2007), LMDZ4 (Risi et al., 2010, Risi et al., 2013), MIROC (Kurita et al., 2011), CAM (Lee et al., 2007) and MPI-ESM-wiso (Cauquoin et al., 2020). The GISS, LMDZ4, MIROC and CAM data are from the Stable Water Isotope Intercomparison Group, Phase 2 (SWING2) (Risi et al., 2012). $\delta^2\text{H}_{\text{seawater}}$ in MPI-ESM-wiso has been calculated from $\delta^{18}\text{O}_{\text{seawater}}$ and d-excess outputs”.

I. 177 and many others: I do not understand the reference IAEA, 2006. All GNIP data should be mentioned with the reference IAEA, 2023.

We corrected the reference to IAEA, 2023.

I. 181-182: why the authors did choose these stations, and not others like Vienna? What are the requirements (e.g., number of consecutive years with data)? How did they make the composite (I mean on which period or on how many years)?

We chose specific stations that are representative of various climate conditions (northern Atlantic, eastern Mediterranean, South Africa and South America). We could have used Vienna station like presented in Figure 2 below, as any other station where the isotopic composition has been reported for a minimum of 3 calendar years within the period 1961-2008. To investigate these monthly variations, we used the 100 years model simulation. We then kept the last 10 years and calculated the seasonal mean over this time period. For easier comparison with the data, we normalized the data by subtracting the annual mean and dividing by the standard deviation for each station. This has been added to the main text.

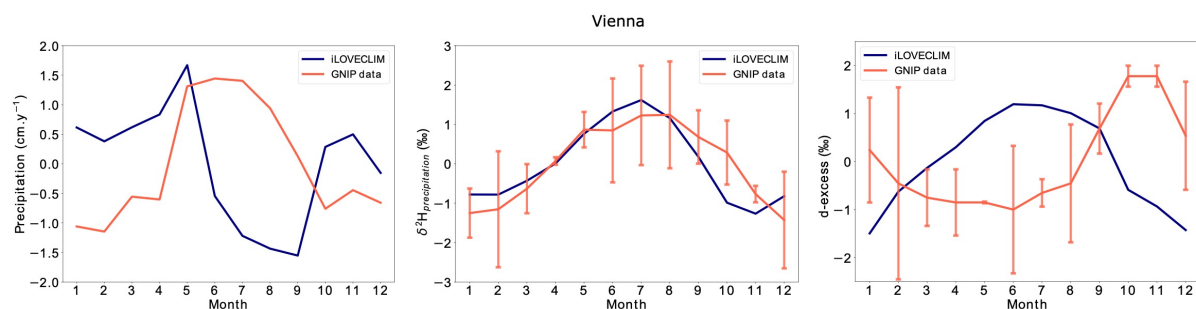


Figure 2: Monthly evolution of the precipitation (left), $\delta^2\text{H}_{\text{precipitation}}$ (middle) and d-excess (right) for Vienna station. The red line is the GNIP data and the blue line is the iLOVECLIM model. The data have been normalized. The error bars for the data are also shown at 2σ .

I. 190-191: You already said in the data section which dataset you will use for the evaluation of your results. You do not need to repeat here again.

We removed it from the text.

I. 193: Please rephrase “Differences with the observations are observed for specific regions.”.

We changed the sentence to “*Regions like central Africa and northern region of South America show however differences with the data since the modelled $\delta^2H_{precipitation}$ is underestimated in comparison to the few measurements available*”.

I. 204-205: I suppose these model results are from SWING2 database. Please add the reference (Risi et al., 2012) and state it clearly.

Yes you are right. We specified that the model outputs used in this study (except the MPI-ESM-wiso and ECHAM5-wiso) come from the SWING2 database and added the reference of Risi et al. (2012).

I. 206: such as strong depletions over Antarctica?

We corrected the sentence.

I. 208- 209: “Similarly to other GCMs, iLOVECLIM shows a small decrease of $\delta^2H_{precipitation}$ and is in the higher range of the observed $\delta^2H_{precipitation}$ values.”

We modified the sentence accordingly.

Sentence at I. 209-210: I do not understand this sentence and it should be removed.

We removed this sentence.

Figure 1 and all the other concerned figures: remove the $\delta^{17}O$, it's not useful, I think.

We moved the $\delta^{17}O$ figures from the main text to the Appendix A.

I. 231-232: please precise what could be these complex processes.

We added the following at the end of the sentence: “*such as the behaviour of the advection scheme at very low moisture content or the role of kinetic fractionation coefficient*”.

Figure 3: is it really useful? I think this figure can be removed.

We removed the figure.

I. 246-247: same comment as for I. 190-191.

Done

I. 253: you say that the model calculates mostly negative values with values ranging from -10 to 10 permil. It sounds a little bit strange, no?

Yes we agreed. We changed the sentence to “*the model calculates values ranging from -10 to 25 ‰*”.

I. 264-265: see my main comment about a fair evaluation of your model results.

I. 272-273: same comment.

I. 289-291: same comment as for I. 190-191. Please explain the possible causes in terms of model biases.

I. 311-313: see major comment about a fair evaluation of the model.

I. 320-321: same comment.

Based on the new figures to evaluate the amount effect, temperature effect, continental effect and to calculate metrics for iLOVECLIM and other GCMs in comparison to measurements (see response to the first reviewer in Section 1.1), we corrected the text in the manuscript to fairly evaluate the model results against other isotopes-enabled models and the observations.

I. 307: H₂¹⁷O instead of ¹⁷O.

Done.

Section 3.1.4: Why these stations in particular? I know that ¹⁷O-excess is not available in GNIP data (and it should be stated). Is there any data of ¹⁷O-excess in precipitation or in water vapor at seasonal resolution (at least) to evaluate iLOVECLIM? Moreover, the evaluation should be done in a fairer way (again). The uncertainties of the data alone do not explain the model-data disagreements.

We chose stations that are representative of various climate conditions (see previous response). We added a sentence in the main text to precise that ¹⁷O-excess data are not available in the GNIP database.

Section 3.2 should be re-organized a little bit for clarification. You can also make separate sub-sections for d-excess and ¹⁷O-excess. Moreover, even if there are no observations ¹⁷O-excess in deep ocean, I would expect to see the results from iLOVECLIM because this is one novelty of this model.

Thank you for this suggestion. We reorganized the Section 3.2 in a new Section 3.3 Isotopes in ocean water, that is separated in two sub-sections for surface seawater and vertical profiles. We also added a new panel on the existing figure of the isotopic depth distribution, to represent the modelled ¹⁷O-excess (Figure 3). With respect to this figure, we added the following text in the revised manuscript: “*The oceanic d-excess and ¹⁷O-excess shows less prominent influence of the main water masses. Above 1000 m, the d-excess goes from 40°S to 40°N with depleted negative values, and enriched positive values for ¹⁷O-excess. Below 1000 m and from 40°S to the north, the NADW d-excess values are higher with a maximum of 2 ‰ around 25°N and 2000 m depth. On the opposite, ¹⁷O-excess values are lower than in the surface, with minimum values at the same latitude and depth than d-excess. The comparison with the δ²H and d-excess observations shows that the model reproduces the depleted surface values and the enriched d-excess values below 1800 m even if the latitudinal gradient is more pronounced in the model than in the data. The depth interval from 500 to 1800 m presents a disagreement between the modelled d-excess and the observation values that are consistently lower than in*

the model. This is especially the case for high latitudes of the northern hemisphere where the difference between the model and the data can reach 2 to 3 ‰. Since no ^{17}O -excess observations exist at depth, we refrain for any further evaluation of the modelled values”.

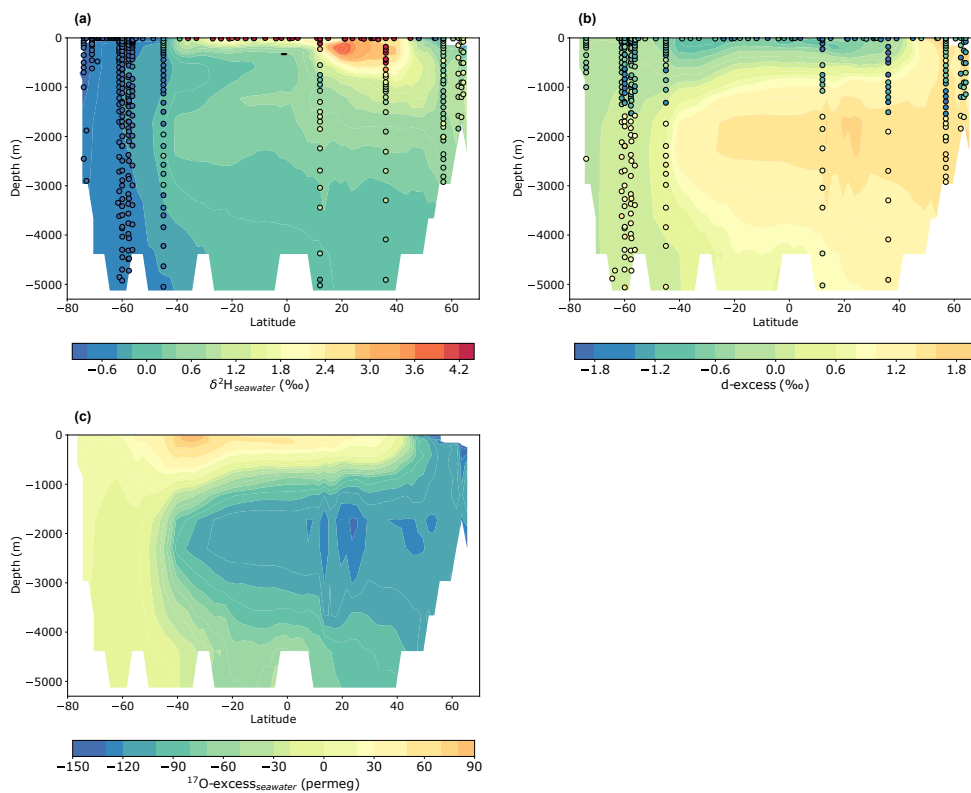


Figure 3: Atlantic zonal mean in iLOVECLIM of (a) $\delta^2\text{H}$ of seawater, (b) d-excess of seawater and (c) ^{17}O -excess of seawater compared to observations.

I. 361-362: you should say that in the observation data section.

I. 370-371: it should be in data section.

We moved these two parts to the Section 2.4 Observational data and water isotopes enabled GCMs.

I. 371 and 372: replace MPI-ESM by MPI-ESM-wiso. Do it also in the legend of the concerned figures.

Done.

I. 387-388: It's one explanation. Usually, very depleted $\delta^{18}\text{O}$ or $\delta^2\text{H}$ values in seawater in Arctic area are explained by the very depleted river discharges. What about iLOVECLIM? If it is not modelled, it is one very plausible explanation for this bias.

iLOVECLIM does not model the river discharges. So it could indeed be one explanation for the enriched isotopic values obtained in the model. We added this hypothesis in the main text.

I. 406: I would say instead that model d2H values are lower than the observations by several permil.

We changed the sentence accordingly.

I. 434: “we presented the implementation of the $^1\text{H}^2\text{H}^{16}\text{O}$ and H_2^{17}O isotopologues in the ...”

Done.

End of line 435: remove “also”.

Done.

I. 439-440 and 443-445: see main comment about the evaluation of iLOVECLIM results.

Following your previous comments, we changed the text of the conclusion that now reads: *“For the atmospheric part, we found a good agreement between the model, the GNIP data (considering the intrinsic biases of iLOVECLIM that could lead to local inconsistencies) and several GCMs, with the conservation of the latitudinal gradient. The modelled $\delta^2\text{H}$ and $\delta^{18}\text{O}$ also fit with the global Meteorological Water Line and the main isotopic effect (amount effect, temperature effect and continental effect are well reproduced in the model). The d-excess distribution for the atmosphere is also correctly modelled at global scale in comparison to the observations and several GCMs. The isotopic composition of oxygen and hydrogen over Antarctica present however differences of several permil in comparison to the data because of the complexity of the local processes at play that are simplified in the model. At present, our models-data comparison suggests that iLOVECLIM does not correctly reproduce the ^{17}O -excess and has a too important dispersion of the values. Modelling the ^{17}O -excess has to be improved in the future versions of the isotopes-enabled models. New measurements are also needed with a reduction of their associated uncertainties”*.

Figure A1: it should be in the main text.

We moved this figure and related text in the Section 3.1.2.

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