Manuscript " Modelling the water isotopes distribution in the Mediterranean Sea using a high-resolution oceanic model (NEMO-MED12-watiso-v1.0): Evaluation of model results against in-situ observations"

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Reply to reviewers' comments

Dear Pr. I., Andrew Yool

We would like to thank you for providing us the opportunity to revise our manuscript, and we are extremely grateful to Pr. Antje Voelker, Pr. Allegra N. LeGrande and the anonymous reviewer for their careful reading and comments that helped to improve our manuscript significantly.

We have revised our manuscript and provided a detailed response to each reviewer's comment and request below.

Color code

Reviewer comments

Authors response

The modifications performed in the manuscript appear in red above and in the revised manuscript with Changes Marked.

Anonymous Referee #2

General comment

Ayache et al. present the implementation of stable water isotopes (d18O and dD) in the high-resolution regional ocean model NEMO-MED12. The simulation of such isotope proxies in climate models is very useful for past climate reconstruction and to better understand climate processes recorded in the water cycle. Ayache et al. performed a simulation for present-day conditions and evaluate their results with available isotopic observations in seawater and marine calcite. They also investigate the relationship of isotopes with salinity. There are not so many studies on isotope modeling in the ocean, even more in a regional model. Moreover, the Mediterranean Sea is interesting in several points of view: many data, a strong east-west contrast in oceanic evaporation, a relatively short residence time… The article is easy to follow, and the analyses are sound. The figures could be improved, especially the used color scales, and some details on the description of the simulation are missing. Moreover, the discussion section is not really a discussion, yet, but more a summary of the results. After addressing these minor points, detailed below, the article of Ayache et al. could be published in GMD.

We extend our thanks to Reviewer #2 for their valuable comments and suggestions, which have contributed to clarifying the manuscript, reinforcing our arguments, and enhancing the main message we aim to convey. The majority of the comments have been incorporated into the revised version.

Specific comments (rather minor revisions)

- Some details on the simulation are missing. Especially, what is spinup time? How was it performed? On line 154, it is said that LMDZ-iso simulation outputs for the period 1990-2020 were used as isotope boundary conditions? What does it mean exactly? That the authors performed a simulation 30 years between 1990 and 2020 with the forcings of the corresponding year? Or that the authors used a climatological average of the LMDz-iso 1990-2020 simulation as boundary conditions, in order to perform a simulation of several decades (so with the same conditions all along the simulation)? What does it involve in terms of bias in isotopic modeled results compared to the observations?

Thank you for pointing this out to us, and we agreed on the importance of clarifying our experimental design.

Here, we used the offline coupling mode. In this method, the physical variables i.e., the circulation fields (U, V, W) and mixing coefficients (Kz) are previously computed by the NEMO-MED12 dynamical model for the 1958–2013 period (Beuvier et al., 2012a) and used to propagate the passive tracers in the ocean.

The simulation was run during 30 years after 44 years of spin-up (1958–1980 repeated two times) allowing us to stabilize the model state (for more than 75 of run). The hydrodynamic forcing has been built from a random draw of year among the historical period (1958–2013 period, Beuvier et al., 2012a) to minimize the impact of the intense events of variability like the EMT or the WMT (Roether et al., 2006; Schroeder et al., 2008). The spin-up strategy was adapted in our previous passive tracer simulations (e.g. tritium and neodymium: Ayache et 2015a, 2016).

The isotopic simulation is performed using outputs from the global atmospheric model LMDZ-iso (Risi et al., 2010b) with an AMIP (Atmospheric Model Intercomparison Project) simulation from 1990 to 2020. The aim is to assess the model's performance in the present climate and against in-situ data observed randomly over the historical period. Therefore, we have opted to use the climatological mean of the LMDZ-iso 1990-2020 simulation as boundary conditions. This decision was made to minimize the warming trend during this period and to ensure that the precipitation and evaporation simulated by the LMDZ-iso model for the current climate situation are as close to the average state as possible, with minimal impact from inter-annual variability.

These points are clarified in the revised manuscript (see section 2.2, lines 149-154).

"The simulation was run for 30 years after 44 years of spin-up (1958–1980 repeated two times) allowing us to stabilize the model state (for more than 75 of run). The hydrodynamic forcing has been built from a random draw of the year among the historical period (1958–2013 period, Beuvier et al. (2012a) to minimize the impact of the intense events of variability like the EMT or the WMT (Roether et al., 2006; Schroeder et al., 2008). The spin-up strategy was adapted in our previous passive tracer simulations (e.g. neodymium and tritium Ayache et al. (2015a, 2016))"

- Still about the experimental design, one important aspect for the calculation of d18Ocalcite from modeled d18Osw is the forcing for surface temperature conditions. As said by the authors, the surface temperature conditions do not come from LMDZ-iso but from an ERA-40 relaxation term applied to the ARPERA heat flux. It means that inconsistencies between d18O of freshwater fluxes and temperature are possible. Could the authors elaborate on this aspect? Could they evaluate the potential biases on the ocean temperature and so on the modeled d18Ocalcite?

Thank you for pointing this out. The reviewer is correct, the forcing of surface temperature used in the calculation of $\delta^{18}O_c$ does not come from LMDZ-iso but from an ERA-40 relaxation term applied to the ARPERA heat flux. This is certainly among the limitations of the OFFLINE coupling mode with the use of a pre-calculated dynamical field.

We presented horizontal temperature maps used in calculating $\delta^{18}O_c$ (refer to Fig. 10c). We checked that this simulation produced reasonable temperature patterns in the Mediterranean Sea against observations. A notable difference arises when comparing the $\delta^{18}O_c$ calculated with high-resolution simulated temperatures (cf. Fig. 3a and 3b below) to that derived from a global model temperature from a global version forced by LMDZ (cf. Fig. 3c and 3d). The global model shows a significant bias in $\delta^{18}O_c$ as a consequence of low temperatures simulated in the Mediterranean Sea (cf. Fig. 3c and 3d).

Additionally, in this simulation, we employed the same freshwater forcing (from Ludwig et al., 2009, and the RivDis dataset, Vörösmarty et al. 1996) as that used in the dynamical simulation (in Beuvier et al., 2012) where the temperature was simulated, ensuring complete consistency between freshwater flux and temperature. This validates our decision to utilize temperatures simulated by the MED12 model and forced by ERA5 rather than the global LMDZ model (see Fig.3 below). However, this inconsistency requires further investigation within a fully coupled ocean-atmosphere model to ensure consistent simulation of changes across various model components.

These points are clarified in the revised manuscript. see Appendix B and the following text (lines 341-343 in the track changes version).

"In this study, we analysed the impact of temperature on $\delta^{18}Oc$ calculations, both in a global model and at high regional resolution. Please refer to Appendix B for further details."

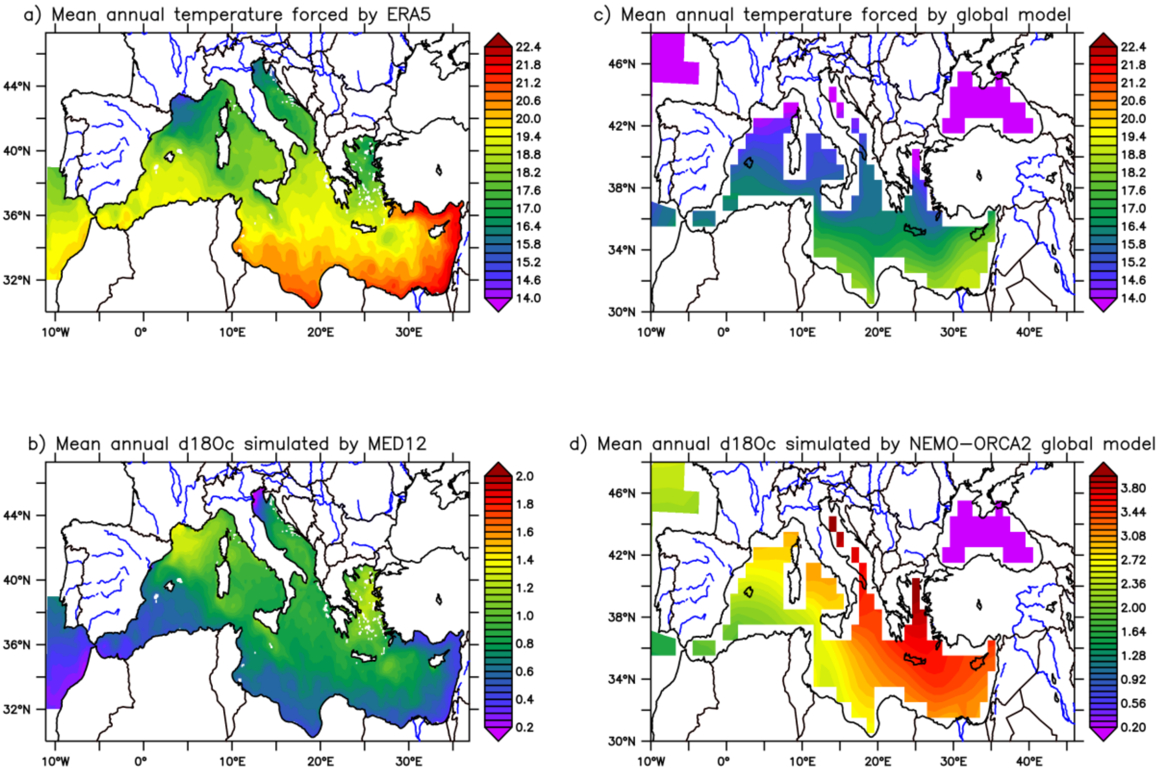

Figure 3 comparing the $\delta^{18}O_c$ calculated with high-resolution simulated temperature (cf. panel a and b) to that derived from a global model using temperature data from LMDZ (c and d).

- The discussion section is not really a discussion but more a summary of the results at the current state of the paper. Here are some topics the authors can discuss: How are the results NEMO-MED-wiso compared to global ocean models or coupled models? Are they improved thanks to the high resolution of NEMO-MED-wiso? The authors talk about coupling as a perspective, but what is possible to do with this model given that it is a regional model, not a global one? How can it bring new useful insights for paleoclimate applications except by putting as boundary forcings the atmospheric fields from paleoclimate global simulations (i.e., offline)? Can this model be used to improve global climate models? The seasonality aspect on d18Ocalcite is interesting, could you elaborate more on this aspect?

Thank you! We think that these points raised by the reviewer are very important to enrich the discussion and the perspectives of this work. We have included these various points in the new version of our paper:

#How are the results NEMO-MED-wiso compared to global ocean models or coupled models?

The model's high resolution presents a unique opportunity to represent a realistic thermohaline circulation in the Mediterranean basin, thus enabling a better understanding of the processes governing water isotopic distribution within this intercontinental basin.

We initially discussed the potential impact of model resolution in the submitted version of our paper (refer to lines 337-341). Additionally, within our team, we utilize a low-resolution global NEMO model (ORCA 1° and 2° horizontal resolution). Figure 4 (below) provides a comparison between the results of the global model (ORCA2) and NEMO-MED12 model, using the same water isotopes modeling approach and forced by the same atmospheric model LMDZiso (R96).

The figure demonstrates that the global model produces unrealistically high values of $\delta^{18}O_w$ in the Mediterranean Sea, particularly in the eastern basin ($\delta^{18}O_w > 2$, max 3.3), whereas in-situ data show maximum values of around 2.1 (Gat et al., 1996). This comparison with the global model has been incorporated in the revised version to complement the discussion on the high-resolution impact, as suggested by the reviewer (Added in Appendix C).

"Sensitivity tests were performed to investigate the effect of changing the resolution of the LMDZiso atmospheric model (between R96 and R144) and the oceanic model (between ORCA2 and NEMO-MED12), the results of which are presented in the supplementary material of this paper (see Appendix C)"

See section 3.4 lines 376-389.

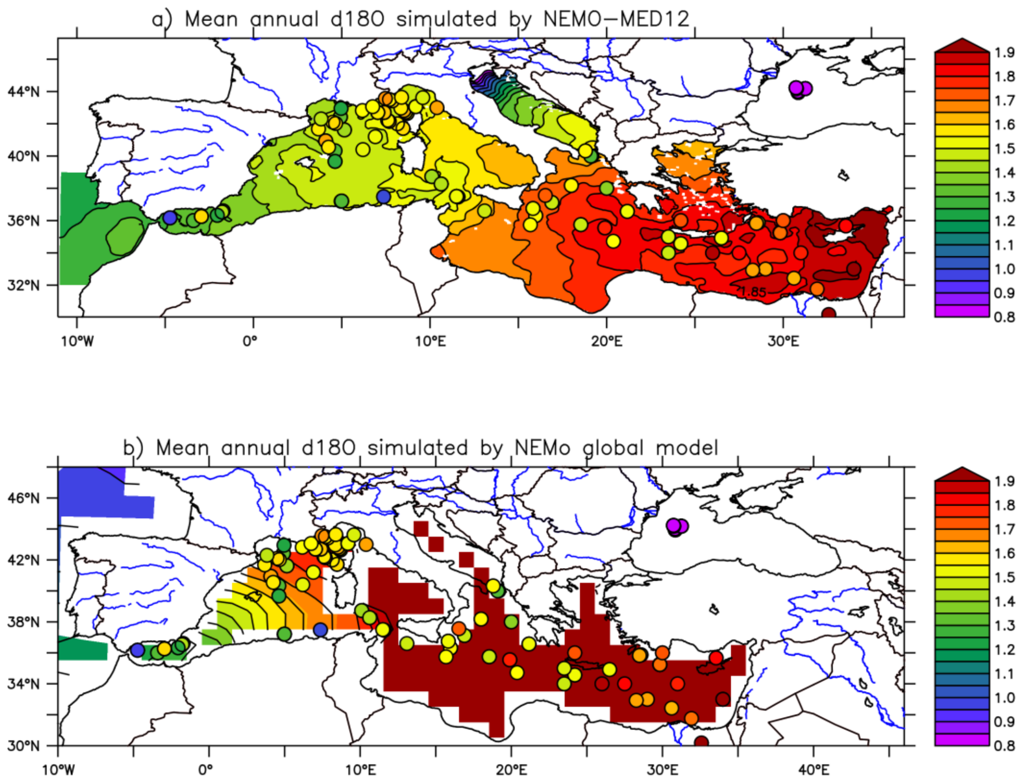

Figure 4 Comparison between the δ18Ow results of the global model (ORCA2 ~2° of resolution) and NEMO-MED12 model, using the same water isotopes modeling approach and forced by the same atmospheric model LMDZiso (R96).

#The authors talk about coupling as a perspective, but what is possible to do with this model given that it is a regional model, not a global one?, #Can this model be used to improve global climate models?

So far, water isotopes have been implemented separately in all components of the IPSL general circulation model (the atmospheric "LMDZiso", soil-vegetation "ORCHIDEEiso" and oceanic "NEMOiso"), but a fully-coupled, isotope-enabled version of the IPSL-GCM is still lacking. A fully coupled simulation will allow us to better understand the feedback and non-linear aspects of the evolution of the water cycle, and hence provide a unique tool for better constraining the past climates simulated in climate models. There is currently a project at IPSL to update the water isotope code in the different components to prepare the isotope-enabled fully coupled version.

Using these models in the Mediterranean region provides a great opportunity to test this water isotope package in a basin where evaporation varies significantly from east to west with a relatively short residence time and much available data. Furthermore, there is no effect of sea ice formation or melting (i.e. no freshwater input from ice sheets during the recent "present situation" period) which is currently not well represented in models. This allows a better understanding of the relative roles of the different parameters within the model and provides a unique opportunity to understand better the spatial and temporal variations of water isotopes for which strict conservation is desirable. Additionally, the water isotope modeling package presented in this study can be utilized in coupled regional configurations of the Mediterranean region, such as regIPSL (refer to https://sourcesup.renater.fr/wiki/morcemed/), which will undoubtedly aid in the preparation of a global-scale coupled version.

We are currently implementing the same water isotopes package, as presented in section 2, into the new global version of NEMO (NEMOv4.2 at ORCA 2° and ORCA 1° of horizontal resolution). This work is aiding us significantly in refining the parameterization of the NEMO global model, particularly in representing runoff forcing. The Mediterranean Sea offers more constrained runoff data/models compared to the global scale, providing insights into the impact of surface runoff. Our sensitivity tests on the influence of the Po River in the Mediterranean Sea, including distributing the Po water discharge across the first vertical levels of the model to prevent numerical instability, have enhanced our understanding. This experience has also enabled us to improve our representation of the Amazon River's discharge in the global version. It’s also important to note that the implementation and effectiveness of such a coupling would likely require further research and validation.

#How can it bring new useful insights for paleoclimate applications except by putting as boundary forcings the atmospheric fields from paleoclimate global simulations (i.e., offline)?

In paleoclimate studies, one major problem with the simulation of past climate changes is that forcings/boundary conditions are not available from observations or data reconstruction to drive high-resolution regional models.

The coupled configuration will make it possible to study past climate for a wide range of periods (i.e. transient simulations) with good confidence, to characterise quantitatively past variations in the isotopic composition of water, and to allow direct comparison between isotopic signals obtained from models and various archives (ice cores, speleothems, oceanic sediment cores, etc.), which is not possible using the offline coupling mode.

Regional climate models can bridge the gap between the coarse resolution of global climate models and the regional-to-local scales. They can provide a more realistic representation of physical processes and climate feedback compared to global climate models. This is particularly true for the Mediterranean region with complex geology. In particular, atmospheric circulation (high wind gusts in winter) and oceanic circulation (deep convection) are better represented in regional models (Ludwig et al., 2019). Also, a numerical platform of global-to-regional modeling has been developed by Vadsaria et al., (2020). This sequential platform may be applied to a large number of paleoclimate contexts from the Quaternary to the Pliocene with regional model forced by a global model. This can be useful for paleoclimate applications, as it can help to answer fundamental paleoclimate research questions and may be key to advancing a meaningful joint interpretation of climate model and proxy data (Ludwig et al., 2019).

We have included additional sentences to better clarify this point in the revised manuscript (see section 4, lines 453-461)

"Regional climate models can bridge the gap between the coarse resolution of global climate models and the regional-to-local scales. They provide a more realistic representation of physical processes and climate feedback compared to global climate models. This is especially true for the Mediterranean region with its complex geology (Li et al., 2006). The water isotope modelling package presented in this study can be used in coupled regional configurations, such as regIPSL (Drobinski et al. (2012), which may assist in the preparation of a global-scale coupled version. Additionally, a sequential architecture of a global-regional modelling platform has been developed by Vadsaria et al., (2020) using the same dynamical model NEMO-MED. This platform can be used sequentially in a wide range of paleoclimate contexts, from the Quaternary to the Pliocene, with a regional model that is forced by a global model."

#The seasonality aspect on d18Ocalcite is interesting, could you elaborate more on this aspect?

Calcite δ^{18}Oc is widely used in paleoclimate research. Understanding its seasonal variability is crucial for reconstructing past climates. The influence of seasonal temperature variability on $\delta^{18}O_c$ (equation 6) is important, particularly in the Mediterranean Sea because of marked seasonal thermal contrast. The $\delta^{18}O_c$ values are determined by both $\delta^{18}O_w$ and the seawater temperature at the calcification depth. For planktonic foraminifera such as *Globigerinoides ruber* and *Globigerina bulloides*, the calcification depth typically ranges from 0 to 100 meters, though variations exist depending on the basin (De Castro Coppa et al., 1980; Grazzini et al., 1986). The season of maximal foraminiferal production can be estimated by data from sediment traps. For instance, *G. ruber* and *G. bulloides* have been associated with calcification seasons in October-November and April-May according to Kallel et al. (1997), while others suggest January-March (Avnaim-Katav et al., 2019) and February-April (Rigual-Hernandez et al., 2012).
In this context, we used our model results to explore the relationship between $\delta^{18}O_c$ and temperature. We employed a paleotemperature equation for inorganic calcite by Kim and O'Neil (1997), which was modified by Bemis et al. (1998), as shown in Fig. 10. Our simulations indicate that the highest $\delta^{18}O_c$ values occur during winter (February, March), while the lowest values are observed during summer/autumn. Although the available observational data do not cover all months of the year, our results align with existing data, highlighting the significant influence of temperature on δ^{18}Oc in the Mediterranean Sea. Nonetheless, a dedicated study should be conducted to further elucidate the seasonal aspect.

In the revised version of our paper, we have included additional sentences to provide clarity on the seasonality aspect of $\delta^{18}O_c$ (see section 4 lines 427-441).

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- The green-to-red colormap used in several figures is not appropriate for colorblind people and should be changed.

Thank you for pointing this out. The same point has been raised by the first reviewer. In the new version of the paper, the colour palettes have been changed.

- The d18Ocalcite dataset is not described in the method section (section 2.5).

The $\delta^{18}O_c$ data were recalculated employing present-day $\delta^{18}O_w$ and temperature data cited in this paper (in section 2.5). We utilized the same paleotemperature equation applied to model outputs, as described by Kim (1997) and further refined by Bemis (1998) for inorganic calcite. Comparison with real paleo data was not conducted as our simulations and their associated forcings were designed for the present-day situation; a specific paleo simulation was not undertaken in this study.

Clarified in the revised ms (see section 3.4, line 325)

"The equation was applied to both the model output and the available in-situ data, as presented in Section 2.5"

- The difference between R96 and R144 is described very briefly. To show the difference map between R144 and R96 for both d18Osw and applied isotope freshwater fluxes could help to understand better what does (not) happen. Could the remapping from LMDZ-iso grid to NEMO-MED-wiso one partly explain this non-diff erence? See technical comments below.

We have performed some sensitivity tests of the results by changing the horizontal resolution of LMDZ-iso between R96 and R144. The results are very close to each other as shown in Fig. 6. It is possible that there is a certain threshold of spatial resolution below which the simulation is improved by a finer resolution. Vadsaria et al. (2020) showed that high resolution (~ 30 km of the atmospheric model with a more realistic wind pattern and hydrological cycle) is critical to accurately capture the synoptic variability needed to initiate the formation of the intermediate and deep waters of the Mediterranean thermohaline circulation (Li et al., 2006). Therefore, we decided to work with the R96 resolution which is the least expensive.

Following the suggestions made by the reviewers, we have included a figure 5 below showing the $\delta^{18}O_w$ anomaly map between the two simulations R144 and R96. The difference between these simulations is minimal, ranging between -0.2 and +0.2 ‰. One possible explanation for this slight difference lies in the runoff forcing utilized. As explained in the manuscript, the runoff forcing is derived from data by Ludwig et al. (2009) rather than from LMDZiso. This is because the water flows simulated by LMDZiso are unrealistic in the Mediterranean basin (e.g., LMDZiso significantly overestimates the Nile river discharge).

To sum up, the change of horizontal resolution between R144 and R96 is not sufficient to generate drastic changes in evaporation and precipitation (as suggested by Vadsaria et al., 2020). The fact that the same runoff forcing was used in both the R96 and R144 simulations explains the small difference between these two simulations.

We have moved Figure 6 to the supplementary materials because this change in resolution does not significantly impact our results and could potentially dilute our main message, and the following text was added in the revised version

"Sensitivity tests were performed to investigate the effect of changing the resolution of the LMDZiso atmospheric model (between R96 and R144) and the oceanic model (between ORCA2 and NEMO-MED12), the results of which are presented in the supplementary material of this paper (see Appendix C)."

(see lines 376-379 and appendix C).

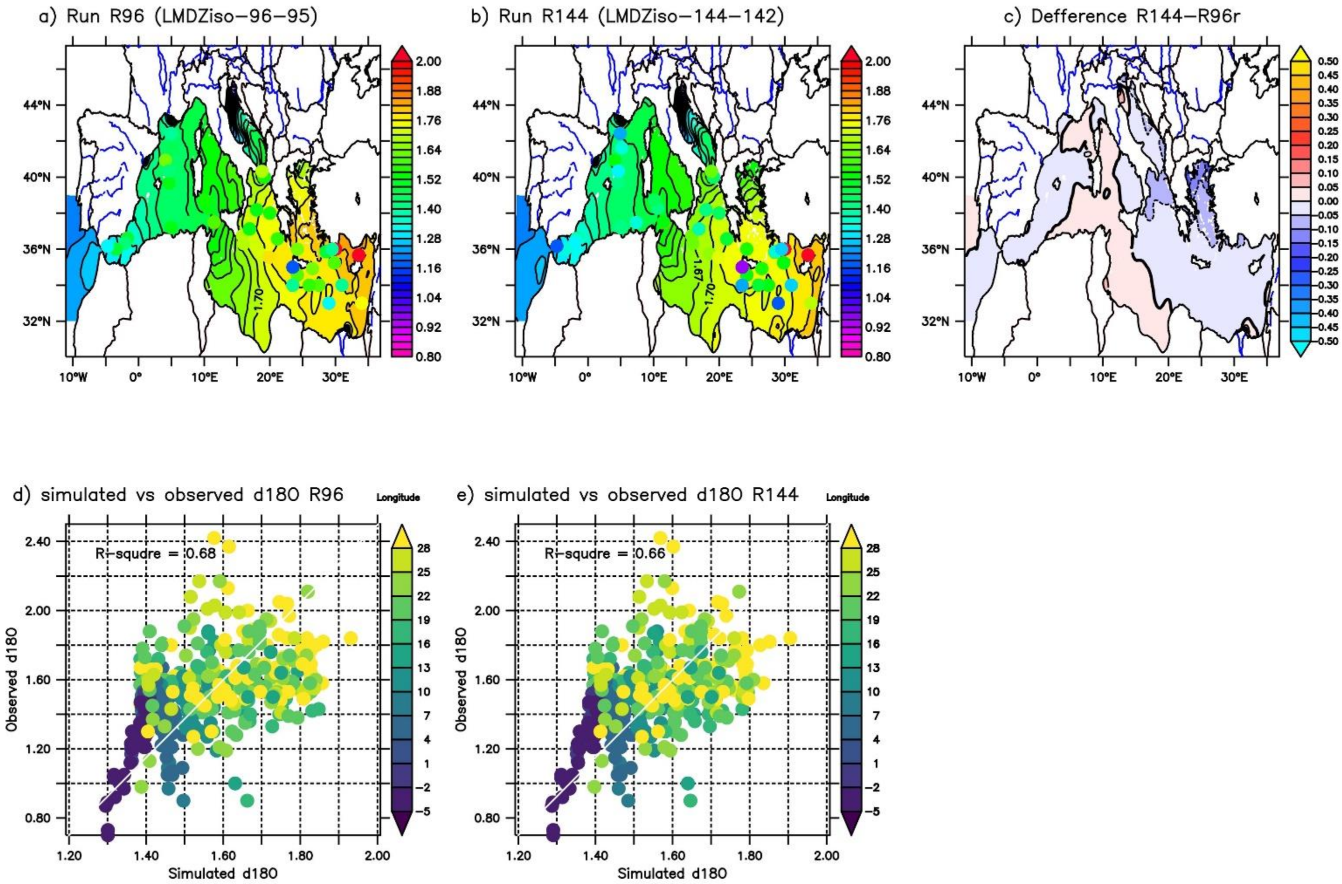

Figure 5 Distribution of $\delta^{18}O_w$ (in per mil) in surface water (at a depth of 50 m) from the R96 simulation. Colored dots represent in-situ observations compiled from Epstein and Mayeda (1953), Stahl and Rinow (1973), Pierre et al. (1986), Gat et al. (1996), and Pierre (1999). Panel d) presents a multi-scatter plot comparing simulated $\delta^{18}O_w$ (averaged over the last 30 years of the simulation) from the R96 simulation with in-situ data from the mentioned sources across the entire basin. The color code indicates the latitudes of the data in degrees east. Panels b) and e) depict the same as panels a) and d), respectively, but from the R144 simulation. Panel c) illustrates the $\delta^{18}O_w$ anomaly map between the R144 and R96 simulations in surface water

Minor technical comments:

- Line 14: O is missing in d18O.

  Corrected

- Line 16: (d18O-S relationship) can be removed.

  Done

- Line 40: "high resolution regional ocean model, yet.".

  Added

- Line 57: Replace that by which.

  Replaced

- Line 67: remove "as an oceanographic tracer".

  Removed

- Line 76: We use isotope fluxes from…

Changed

- Line 110: The term isotopologue should be used at the beginning of the paper (line 14). Then you can say you use the term isotope instead.

Agreed

- Line 110: high-resolution

Corrected

- Line 121: replace bouquin AIEA by the appropriate IAEA reference.

Changed

- Lines 142-143: Table S2 are…

Corrected

- Section 2.3: see major comment about spin-up time and simulation length.

In the revised version of the paper, more information has been added about our experimental design (see new section 2.2).

- Line 157: remove Risi et al., 2010b.

Done

- Section 2.5: see major comment about the description of d18Ocalcite dataset.

The information was added in the revised version

- Line 230: pseudo-salinity results or standard modeled salinity?

Pseudo-salinity (corrected)

- Section 2.3: please change salinity by pseudo-salinity where needed to avoid misunderstanding between the modeled standard salinity of NEMO-MED and the pseudo-salinity described in this paper. Change salinity by pseudo-salinity in the title too.

Thank you for pointing this out. Changed in the revised version.

- Line 238: spatial slope?

Indeed. Added

- Line 241: between observed salinity and d18Osw…

Added

- Lines 259-265: this part has nothing to do with the d18O-pseudo salinity relationship. It should be removed, except if you can show a change in the relationship when using R96 or R144 LMDz-iso fields.

Thank! We have added a comparison between standard simulated salinity and pseudo-salinity (see new Appendix D)

Overall, the pseudo-salinity globally yields values highly comparable to standard simulated salinity. Minor deviations are noticed in the Gulf of Lions and the Algerian

Basin, attributed to overlooked mesoscale activity impacts in the global LMDZiso simulation.

- Section 3.3: I think the part on dD can be removed. It's similar to d18o and there are not so many data. Figure 7 should be removed too.

We agree with the reviewer that δD_w and $\delta^{18}O_w$ tendencies are similar since identical boundary fluxes (precipitation, evaporation, and river runoff) drive both $\delta^{18}O_w$ and δD_w isotopes in the surface water. However, as this is a development paper, we have included the deuterium results to show that the code exists and can be used by the scientific community. Besides, simulating and evaluating both δD_w and $\delta^{18}O_w$ is necessary for the perspective of the future coupling of NEMO with the other components of the IPSL model, which will be used for paleoclimate applications involving both δD and $\delta^{18}O$ of natural archives. In particular, δD in leaf waxes (Sachse et al 2012) and speleothem fluid inclusions (van Breukelen et al 2008) are useful for paleoclimate reconstructions.

We have clarified this point in the article: "Simulating both δD_w and $\delta^{18}O_w$ is useful for paleoclimate applications involving both δD and δ18O of natural archives, particularly when using this modelling approach in a fully coupled configuration. Notably, δD in leaf waxes (Sachse et al., 2012) and speleothem fluid inclusions (van Breukelen et al., 2008) are useful for paleoclimate reconstructions."

See section 4, lines 418-420 in track changes version

- Lines 266-277: can be removed.

We prefer keeping the δD result, because of its relevance for paleoclimate reconstructions as explained above.

- Line 278: remove (d-excess= δD - 8* δ18Osw, Dansgaard, 1964) as you already said it at the beginning of the paper.

Done

- For the Figure 9, it could be interesting to see the depth profile of d-excess too. Are there some data to compare with in EMed (according to Figure 7)? Then you could maybe elaborate a little bit more for the section 3.3.

Thanks to the suggestion of the first reviewer we have found new dD and d-excess data in the western basin (Reverdin et al., 2022) and we have added these data to Fig. 7. The data have allowed us to replot Fig. 9 and enrich the discussion of the section 3.3.

See the new figure below and the new section 3.3 in the revised version.

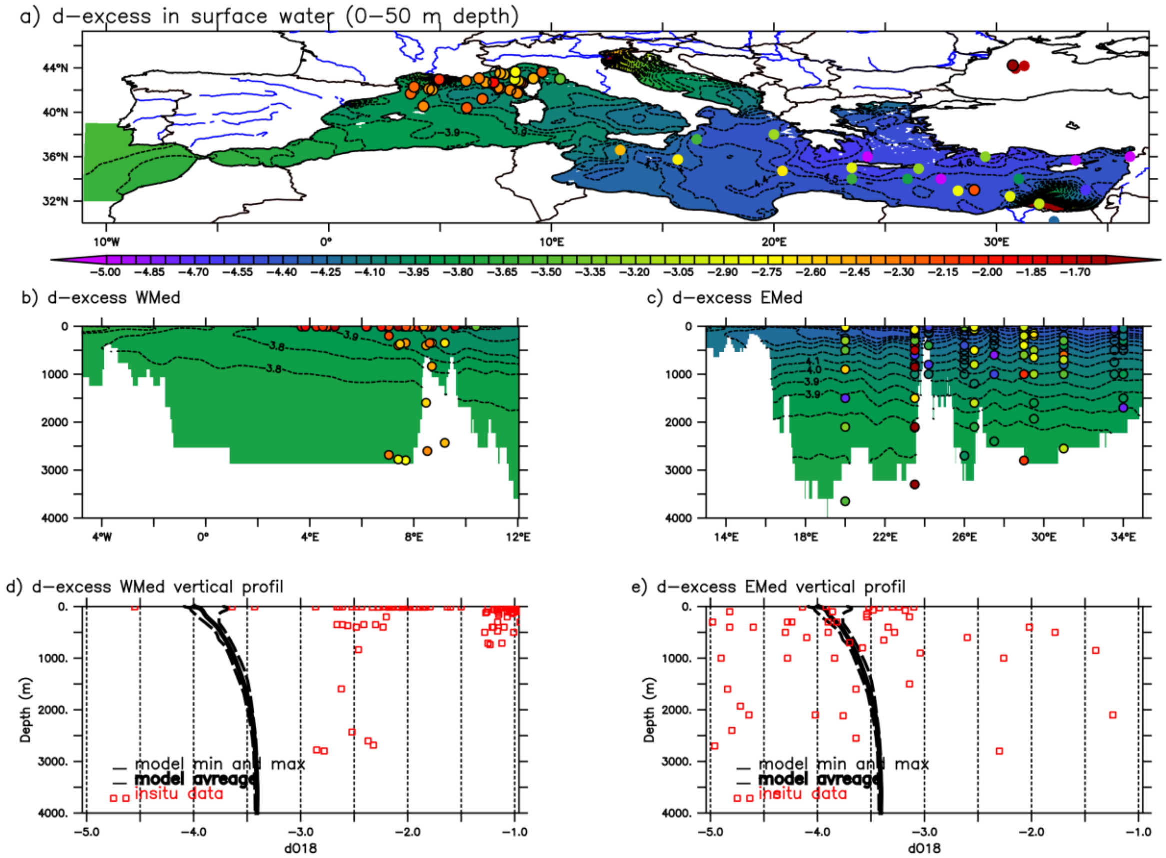

Figure 6 The model outputs against in-situ data for the present-day situation. a) d-excess (in ‰) distribution in the surface water (50 m depth). b) E-W vertical section of d-excess (in ‰) in the western Mediterranean basin d) Zonal mean comparison of d-excess (in ‰) average vertical profiles in the western basin presenting model results against in-situ data. c) and e) the same as b) and d) but for the eastern basin. Colour filled dots represent in-situ observations from (Gat et al., 1996; Reverdin et al., 2022). Both model and in-situ data use the same colour scale.

- Figure 1: typo in "Precipitation" in plots d, e, and f. Also in the legend of the figure.

  Done

- Figure 6: could you show the difference R144-R96 in the d18Osw, but also in the applied isotope freshwater fluxes. It could help to understand the little difference between the two simulations and to elaborate a little bit more (for now, the results are described in 6 lines at the wrong place (lines 259-265).

  In the revised version of our paper, the text (lines 259-265) and Figure 6 has been moved to the supplementary materials (Appendix C) as this change in the resolution doesn't significantly affect our results and could potentially obscure the main message (see Figure below).

  For an explanation of the slight variance between R144 and R96, please refer to our answer to specific comments of the reviewer #2.

- Figure A1: Apply different scales for EMed and WMed d18Osw.

  Done

- Legend of figure A2: average vertical profiles.

Done

References

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