

Interactive comment on “From climatological to small scale applications: Simulating water isotopologues with ICON-ART-Iso (version 2.1)” by Johannes Eckstein et al.

Anonymous Referee #3

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In their paper, Eckstein, J. et al. present a general circulation model that has now been equipped with the water isotopologues HDO and H₂¹⁸O. It comprises a model description and an evaluation with respect to precipitation, satellite data and in-situ aircraft measurements. Moreover, a “tagged water” concept is presented that can be used for process studies.

Essentially, the paper presents an endeavour that had been conducted numerous times before, a lot of (more than 10) GCMs comprise water isotopologues. Recently, technical advances have been made with respect to advancing and extending the implemen-

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tation of water isotopologues in GCMs or ESMs, e.g. Xu et al. 2012 have integrated the isotopologues in a coupled global ocean model, Haese et al. 2013 have included water isotopologues to a coupled atmosphere-land surface model, Eichinger et al. 2015 have added stratospheric methane oxidation effects. This paper here, however, does unfortunately not include anything novel. Also the evaluation with respect to precipitation and to satellite measurements had been conducted before with other models, in part even in extensive model intercomparison projects (SWING). There are also mistakes in the model conception (surface), but see below at my major comments.

The usage of CARIBIC data for comparison with an isotope enabled GCM is indeed new and interesting, this part of the paper unfortunately is very disappointing. First, it is not well structured, it seems like the authors want to compare everything at once here, instead of doing it point by point and thus no clear message shines through. Second, the evaluation should be much more quantitative and several points should be discussed in more detail here. And third, the method of the model-data comparison with respect to the simulation setup is not suitable for the given goal of the study. See more details on this in the major comments section.

The tagged water concept is a nice tool for process studies, but the concept a) is simple and does not need a reference in GMD, b) has also been implemented many times before and c) is sort of detached from the rest of the paper and d) does not provide any important insights here. More details in my major points.

Moreover, the manuscript requires a general polishing of language and formulations, it is written in a somewhat halting manner with errors and inaccuracies. I provide some examples below in the minor comments and technical sections.

Altogether, I do not think that this paper adds considerable value to water isotope model development. In my opinion, a work that only repeats what had been done before with yet another model, should rather find its place in a short method section, or in the supplement of the paper of another journal, along with an in-depth research study

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using the new tool and answering the one or the other science question. Anyway, although the paper is really disappointing, I guess it is still valid to publish such an article in GMD just to have a reference (if that is what GMD wants), but at least the points I am making below should be considered before publication.

Major comments:

- There are two serious flaws in Section 2.3 that have to be corrected for to achieve a state-of-the-art water isotope enabled GCM:
 - The authors are mistaken when they think that R_{surf} is approximated by R_{VSMOW} in Werner et al., 2011. In ECHAM5-wiso, the surface reservoirs soil, skin, snow and plant layer are filled by precipitation and form R_{surf} , which is then used for evaporation processes from the surface. Only fine processes like isotope fractionation during evapotranspiration are neglected. Using R_{VSMOW} for the entire surface is a step backwards in global water isotope modelling.
 - Also as a lower boundary condition for the ocean, this is not a state-of-the-art approximation and it is not done this way in recent models. Instead, a global gridded data set based on the ^{18}O isotopic composition in sea water by LeGrande and Schmidt, 2006 (see attached figure) is taken e.g. in Werner et al., 2011. HDO in the ocean surface layer can be approximated from this.
- P6L5-6: Wrong. In fact, during freezing of water isotopic effects occur in a closed systems (Souchez and Jouzel, 1984) and there is even evidence of a kinetic effect (Souchez et al. 2000), but due to the comparably low diffusivities in liquid water these effects can be neglected in cloud processes in GCMs. This has to be mentioned somewhere, such inaccuracies should not make their way into scientific literature.

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- Fig. 2 and Sect.3.2: You forgot to include a station in the tropics. Other processes (amount effect,...) become important here that have to be evaluated.
- The simulation setup and the initialization procedure is not suitable for the given goal of the study. To have a one-to-one comparison of water isotopologues in model results and observations a free running simulation with such short spin-up from such a crude initialisation is not applicable, but let me make these points one by one:
 1. Since your aim is to evaluate your representation of water isotopologues (including the water cycle processes as well as fractionation effects) in the model and not the model meteorology, you first have to compare a nudged (specified dynamics) simulation. Otherwise you will never be able to separate the effects of an unequal meteorological situation with the water and isotope effects. And that is what you need to do in the first step, because only then you can really assess your water isotope implementation. Or the other way around, your evaluation is pointless with the used simulation.
 2. In particular with such a crude initialization of HDO, you need longer spin-up time, maybe a month or more. Then you will not face problems like in P21L31, so why not just do it? However, probably already the HDO field of your first simulation could serve as a (somewhat better) initialisation field for your second simulation.
- As mentioned above, the section on the comparison with CARIBIC data should be comprehensively restructured. Comparisons should be made point by point and clear conclusions should be drawn and presented out of that.
- This brings me to my next point. The authors correctly write, that water isotope modelling is applied to answer climatological questions and (this should be "and" not "or" on page 2, see other REF) process understanding. This usually means the simulation of a particular phenomenon for in-depth analysis with the additional

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information from the water isotopes. Here, the authors are using the tool in a weather prediction setup, but they never clarify why they chose this configuration, i.e. how one could profit from this sort of "weather model setup". Or in other words, what advantages does this setup have over the application of the isotopes in a regular climate model configuration.

- The concept of the tagged water tool is simple and it has been developed many times before (which the authors do not even mention), see REF#2. Thus, the concept itself does not require another reference in GMD. The process studies that are conducted with it in this paper do not provide any new insights into the hydrological cycle. Plus, there is only little connection of it to the actual topic of the paper, the only real connection is that one can approximate the spin-up time with the approach. This, however, the authors will not need anymore if they consider my point on the simulation setup (which is crucial for the evaluation and thus for the entire paper). Hence, this part of the study dangles somewhere in the nowhere here and should thus be removed completely from the paper.

Minor comments:

- P1L6: This sentence needs to be rephrased, it is incorrect English and it is not clear how this shall represent a range of temporal scales.
- P2L7-9: This sentence is grammatically wrong (dangling participle).
- P2L26 and elsewhere: Cauquoin and Risi, 2017 has been rejected by GMD. You may want to find another citation for this.
- P2L31: Most (if not all) models can be run with a fine horizontal resolution. How does the ICON model "stand out" from other models with respect to this?

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- P2L32: You use the word "flexible" here and also later on in the paper, and I think the word is being misused here. A model is not flexible when you can implement a lot of diagnostics, or run several water tracers at once. Basically you can do that with every model. Flexibility would be for example when you can easily switch these diagnostics and tracers on and off or change their attributes without having to recompile. Or being able to expand the model system such that you have several co-existing processes (e.g. convection schemes) that can be run with the same executable. I am not aware if this is possible in ICON-ART-Iso, if so you could describe it and use the word flexible, if not, you should rather use the word comprehensive or extensive.
- P2L32: You mention "diagnostic moisture tracers" and "tagged water" here, but at this stage the reader has no idea what you actually mean with that. Either explain it shortly, or wait until it comes to the point.
- P3L2 and L6 and throughout the manuscript: A section does not compare or discuss anything. These formulations make no sense, instead **you** compare it **in** the section. So use e.g.: In this section, we discuss....
- P3L26: And why is this a very good assumption? Because the abundance of standard water is at least three orders of magnitude higher than the abundance of any rare isotopologue. Why not include this in the text?
- P3L27-29: Rephrase: ...seven different forms (vapor, cloud water, ...), each of which is represented by one tracer for standard water and one tracer for the isotopologues HDO and H₂¹⁸O, respectively.
- P4L1: What settings?
- P4L21-22: Sentence is unclear, rephrase.

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- P8L23-24: At this stage, it is totally unclear where the simulation of "tagged water" is supposed to aim at, so this sentence is rather confusing.
- P8L30: and throughout the manuscript: To avoid ambiguity, the δ should be complemented by the isotope, the molecule and if relevant also by the phase, such as: $\delta D(H_2O_{ice})$.
- Sect. 2.7: The text never says that you are using HDO measurements here (only in the table caption), that makes the read unnecessarily confusing
- P9L15-20: This paragraph leaves unclear what this is supposed to be good for, why do you do that?
- P9L22: Please rephrase, the sentence is unclear. Also, why are you doing that?
- Fig. 1: Give panels a,b,c,d,e,f and change text accordingly
- P12L4: 73h is a very coarse output time step. Why so coarse? That makes only 10 steps a month, I think that is too weak if you want a robust climatology.
- P12L5: Why 91.25? Magic number?
- P12L12-13: Shortly explain why you do that.
- P12L27-32: The temperature bias should have a large impact on the isotope ratios. That does not always seem to be the case, see .e.g. Ankara. How come? In the depiction it is hardly possible to see how far the values are off, the vertical axes are too coarse.
- P14L25: Why 90%? Another magic number?
- Sect. 3.3.1: Do you take the model output at the same times and the same locations as the satellite makes observations (overpasses)? For this comparison you should.

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- Fig. 3 and 4: Give panels a,b,c,d and change text accordingly
- P18L4: Two more magic numbers, please explain.
- P19L16-17: That would mean the flights take place in the extratropics only, because in the tropics these altitudes are still the troposphere. The flights do however seem to cross the equator, something is wrong here!
- P19L26: What conditions? Weather in general, or humidity, or what?
- P20L4-5: The flights do not sample the model atmosphere, the flights take measurements of the real atmosphere. Your off-line interpolation of the model data samples the model atmosphere. Be more precise.
Moreover, taking only 1h output for this comparison you should make clear that, with an approximate flight velocity of the aircraft of around 900km/h, you will only get less than 10 model points per flight you are interpolating your data to. That is very coarse given that you are aiming on comparing local phenomena. In fact, it would be better to use an on-line flight tracking tool with high temporal resolution for this.
- Sect 3.4.1: Please state when exactly was which flight.
- P20L7: The hurricane processed your data? Please rephrase.
- P20L8: What model simulation?
- P20L9: What exactly do you mean by "the IAGOS-CARABIC database is examined"?
- P21L1: I do not understand what you mean by "randomly drawn" and "randomly chosen", please explain. If you want to make a climatological comparison here, why not make a long simulation to have a fair comparison?

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- P21L23-24: From this depiction I cannot even see this. You should make the evaluation much more quantitative.
- P21L31: This is one part of what I mean with my major point on the simulation setup. If you had a longer (some months) spin-up time, you would not have to face these problems.
- Fig. 7: What does the N stand for?
- P23L5-8: So if you want to discuss stratospheric intrusions you can not get around methane oxidation and its influence on $\delta D(H_2O)$ in the stratosphere. Depending on from which altitude the air is transported downwards, this could mean strongly depleted or enriched water vapour. Also, work has already been done to parameterize this effect on HDO in GCMs (Schmidt et al. 2005, Eichinger et al. 2015), it is a shame that this is not even discussed here given that you are evaluating results in the UTLS.
- P23L8: "air has been processed by the model" What does that mean? Please rephrase.
- P23L9: "different processes" What processes? At least shortly list some.
- Sect. 4: Change title from "Conclusions" to "Summary (and outlook)", there are no conclusions that go further than what had already been written before.
- P24L10: What do you mean by "long term stability"?

Technical issues:

- P1L18: ...oceans are an unmatched ...
- P1L18: "a reservoir to dissolve" - refine wording
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- P1L12-13: It is not clear what is meant by "all of tropical data" here.
- P2L8: ... isotopologues in **water** vapor ... - this inaccuracy appears several times
- P2L14-15: Refine the english. Suggestion: The isotopologue content of water vapor has first been measured by means of cryogenic samplers (Dansgaard, 1964). In the last 15 years, also laser absorption spectroscopy methods have been developed for that use.
- P3L7: ... with the results of ICON-ART-Iso simulations. (You compare the results, not the simulations)
- P3L14: ... is the water isotopologue enabled ...
- P3L25: To discriminate , unclear, rephrase.
- P3L26: For clarity, you should write $^1H_2^{16}O$ here.
- P4L1: Remove "As".
- P4L17 The parameterization that influence ...
- P4L29-30: The ratio of ratios?
- P4L31 (and throughout the section): Put equation 2 here, not at the end of the paragraph. Generally restructure the presentation of equations.
- P6L6: ilead
- P8L20: ... in the standard setup
- P8L23: initialization of the water isotopologues!
- P9L9-14: repetition

- P9L15 what are water species?
- P9L21 diagnostic
- P13L3: remove "In doing so"
- P18L15: criterion
- P19L8: ... in the tropics serves as reference.
- P19L23: ...resolution is finer than the ...
- P19L24: remove "very"
- P19L28: ... Hurricane Igor had passed ...
- P21L5: laong
- P21L6: deld
- P23L5: show show
- P23L10: ...along the ...
- P23L16: remove "of"

References:

Souchez et al. 2000, A kinetic isotope effect during ice formation by water freezing, GRL, 27:1923:1926

Souchez and Jouzel 1984, On the isotopic composition in δD and $\delta^{18}O$ of water and ice. JoG, 30:369-372

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Schmidt, G. A. et al. Modeling atmospheric stable water isotopes and the potential for constraining cloud processes and stratosphere-troposphere water exchange, JOURNAL OF GEOPHYSICAL RESEARCH, VOL. 110, D21314, doi:10.1029/2005JD005790, 2005

Haese, B. , Werner, M. and Lohmann, G. (2013) Stable water isotopes in the coupled atmosphere-land surface model ECHAM5-JSBACH , Geoscientific Model Development, 6 , pp. 1463-1480, doi:10.5194/gmd-6-1463-2013

Eichinger, R. , Jöckel, P. , Brinkop, S. , Werner, M. and Lossow, S. (2015) Simulation of the isotopic composition of stratospheric water vapour – Part 1: Description and evaluation of the EMAC model , Atmospheric Chemistry and Physics, 15 (10), pp. 5537-5555, doi:10.5194/acp-15-5537-2015

Xu, X. , Werner, M. , Butzin, M. and Lohmann, G. (2012) Water isotope variations in the global ocean model MPI-OM , Geoscientific Model Development, 5 , pp. 809-818 . doi:10.5194/gmd-5-809-2012

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