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Interactive comment on "Kinetic mass-transfer calculation of water isotope fractionation due to cloud microphysics in a regional meteorological model" *by* I-Chun Tsai et al.

Anonymous Referee #2

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In this manuscript the authors present an implementation of the heavy stable water isotope HDO in the National Taiwan University (NTU) microphysical scheme of the Weather Research and Forecasting (WRF) model. Isotopic fractionation during both liquid and ice cloud formation is computed according to kinetic mass transfer principles, which is possible because the NTU scheme does not apply the saturation adjustment technique. The model was subsequently used to study a cold front event in northern Taiwan, and disentangle different mechanisms that led to a decrease of δD in vapor and precipitation. The results show that cloud microphysical processes, the initial vertical distribution of δD, and lower boundary conditions are all similarly important for reproducing the observed evolution of δD during the cold front passage.

This is a well-written and interesting manuscript that takes advantage of the kinetic mass transfer formulation in the NTU scheme to physically simulate isotopic fractionation during cloud formation, avoiding equilibrium assumptions or uncertain parameterizations of supersaturation. The study nicely demonstrates how numerical models can help interpret isotope measurements and improve our understanding of the water cycle also on short time scales. I recommend that the manuscript be published after minor revisions.

General comments

1) The bibliography could be updated with some newer references. For example there are now isotope models that no longer apply saturation adjustment during ice cloud formation, e.g., IsoSAM (Blossey et al. 2010), COSMOiso (Pfahl et al., 2012).

2) As per comment (1) it would be interesting to see an additional experiment (maybe in the supplement) that assumes thermodynamic equilibrium only for the liquid phase, but not for ice. The nonequilibrium effect is generally assumed to be much stronger during ice than during liquid cloud formation due to higher supersaturations. Such an experiment would show how accurate this assumption is, and whether applying saturation adjustment and isotopic equilibrium during liquid cloud formation (as done in the models mentioned above) is reasonable or not.

3) Due to the low diffusivities of water molecules in ice there is no homogenization of isotopes in ice crystals and snow flakes. During deposition, the vapor only "sees" the outermost layer of the ice crystal / snow flake. Could you add a few sentences on how you define the isotopic composition of this outermost layer in the NTU scheme? For example, is it equal to the bulk composition of ice / snow, or the composition of the deposition flux? What is your rationale for one or the other?

4) Supersaturation and associated nonequilibrium effects are especially important for the second-order isotope parameter deuterium excess (d=δD - 8*δ18O) . It would be interesting to see the results of this case study also for deuterium excess, which would,

however, require having H218O in the model. This could be something for a future study.

5) There are some minor English mistakes / typos, which I won't correct here. I suggest to ask someone for proofreading before resubmission.

Specific comments

Line 63: Better "liquid or ice and gas phases". For ice, supersaturation is (presumably) even more important than for liquid.

Line 195: I personally don't like the factor 1000 in the definition of δ, because it is not part of the definition but part of how the definition is expressed. A similar thing would be to define pressure as p = F/A * 0.01 because it is often expressed in hPa. But this is a detail.

Line 207: "the ratio between the HDO concentration (QIV) and QV changes rather linearly with height." I am confused about this sentence. It does not seem linear in Fig. 4b.

Line 260-262: This sentence is not very clear. Do you mean depletion due to rain-out of heavy isotopes? Strong fractionation would otherwise lead to higher δD in the hydrometeors.

Line 283: Better "low δDV" instead of "significant δDV".

Line 304: Do you mean δDI (instead of δDV)?

Line 322: Better "the decrease in δDV was overestimated", because δDV itself is underestimated.

Line 328: For consistency I would also discuss the NoFrac simulation already in the results section.

Line 370: Reference for precipitation measurements?

Line 380: Also evaporation from the ocean can have a large influence on the isotope values close to the surface. As far as I understood, this is not explicitly considered in the model. Is that correct?

Line 403: "overestimate the decrease of δD", or "underestimate δDV".

Line 410: Same as line 403 but the other way round.

Fig. 1: Write out the terms CCN, GCCN, IN in the figure caption.

Fig. 4b: Labels for the axes would be helpful.

Fig. 6: Is this a daily average? Please specify.

Fig. 7: For consistency "observed (OBS: black line)". Rotate time axis labels so they are more readable.

Fig. 10: Figure resolution is bad, labels are small and not readable. Where do you calculate the vertical distribution? Is the x axis in space or time?

Fig. 12: Add units.

References

Blossey, P. N., Z. Kuang, and D. M. Romps (2010). Isotopic composition of water in the tropical tropopause layer in cloud-resolving simulations of an idealized tropical circulation. J. Geophys. Res., 115, D24309, doi:10.1029/2010JD014554

Pfahl, S., H. Wernli, and K. Yoshimura (2012). The isotopic composition of precipitation from a winter storm – a case study with the limited-area model COSMOiso. Atmos. Chem. Phys., 12, 1629–1648, doi:10.5194/acp-12-1629-2012