Review of "Retrieval of $\delta^{18}O$ and δD in atmospheric water vapour from ground-based FTIR"

The paper addresses a field that is well in the scope of AMT. Observations of the ratio between different water vapour isotopologues can contribute to a better understanding of the atmospheric water cycle (climate feedbacks, atmospheric energy budget, cloud processes, etc.).

The authors retrieve total columns of $H_2{}^{16}O$, $H_2{}^{18}O$, and $HD^{16}O$ from near infrared solar absorption spectra. They apply a profile scaling retrieval, i.e. use apriori assumed profiles of $H_2{}^{16}O$, $H_2{}^{18}O$, and $HD^{16}O$ and scale them during the retrieval process. The apriori information comes from daily NCEP/NCAR humidity re-analyses and very simplified assumptions for the relations between the different isotopologues. After the retrieval process the retrieved total column data are used for calculating the columnar ratios $H_2{}^{18}O/H_2{}^{16}O$ (or $\delta^{18}O$) and $HD^{16}O/H_2{}^{16}O$ (δD).

General remarks:

(1) More uncertainty estimations are needed:
Isotopologue ratio data calculated aposteriori from retrieved column data have already been used in scientific studies (model validations, satellite validations, etc.). For instance, $H_2{}^{16}O$ and $H_2{}^{18}O$ columns are made available by TCCON and then used for calculating columnar δD. However, I am not aware of any study that comprehensively investigates the uncertainty of such aposteriori calculated δD values. In this context I was happy to see that the authors discuss the impact of some uncertainty sources. The manuscript discusses measurement noise, uncertainty in the assumed apriori temperature profiles, uncertainty in the apriori assumed relation between the isotopologues, and the uncertainty in the spectroscopic parameters. Unfortunately, the authors forget about a very important uncertainty source, which is the uncertainty in assuming the humidity profile according to the NCEP re-analyses. In Figure 7 the authors estimate how the assumed correlations between the isotopologues can affect the ratio calculations, however, the NCEP re-analyses is a much larger uncertainty source for the apriori profile shape of $H_2{}^{16}O$, $H_2{}^{18}O$, and $HD^{16}O$. The authors should estimate how a 20% uncertainty in NCEP (maybe with a correlation length of the uncertainty of about 2.5km) affects their ratio products.
By extending the uncertainty estimations the authors can make a very useful contribution, since aposteriori calculated ratios are already used for scientific studies, but comprehensive uncertainty estimations are still missing.

(2) Clearer discussion of the differences wrt the MUSICA data is needed:
During the recent years and in the context of the ERC project MUSICA there has been significant progress with retrievals that optimally estimate the $HD^{16}O/H_2{}^{16}O$ ratios from mid-infrared solar

absorption spectra. These ratio retrievals are rather different from the aposteriori ratio calculations as presented by the authors. The authors should make this difference very clear and also mention the large efforts made within MUSICA for documenting the uncertainties of ratio products (similar efforts are still missing for the aposteriori calculated ratio products as presented by the authors).

Detailed remarks:

(1) The title is misleading since the authors retrieve $H_2{}^{16}O$, $H_2{}^{18}O$, and $HD^{16}O$ and not $\delta^{18}O$ and δD! The title needs to be modified accordingly. I propose:
"Aposteriori calculation of $\delta^{18}O$ and δD in atmospheric water vapour from ground-based FTIR retrievals of $H_2{}^{16}O$, $H_2{}^{18}O$, and $HD^{16}O$"

(2) Similar to (1): in the abstract the authors talk about retrieved $\delta^{18}O$ and δD or $\delta^{18}O$ and δD retrievals. I think it is important to make clear that the ratios are calculated after the retrieval process, since the aposteriori calculation is an important error source.

(3) Page 204 last line to page 205 line 2: The authors should not try selling a drawback as an advantage: If you scale a profile, but your spectrum contains information about the profile shape, your result will depend on the assumed apriori profile shape.

(4) Page 205 line 4 and Fig. 5: what is the weighting function? Is it the Jacobian (dy/dx) or the gain function (dx/dy). I am more used to averaging kernels. Maybe it is possible to plot the averaging kernels?

(5) Eqs. (3) and (4): STD between ECHAM and the simplified "model" of Eqs. (3) and (4) is 35‰ and 4‰, for δD and $\delta^{18}O$, respectively. That is you need a precision of 35‰ and 4‰! If you do not reach this precision you don't have to measure δD and $\delta^{18}O$, then you can just calculate it from $H_2{}^{16}O$ according to Eqs. (3) and (4), right?

(6) Page 208, line 20-23: The authors seem not to account for the averaging kernel when comparing to the model? If yes, this should be mentioned.

(7) Page 208, line 27: The authors seem to perform retrievals for each spectral window independently. This is different to what I know from TCCON and NDACC, where all windows are generally fitted simultaneously. Maybe this difference should be made clear.

(8) Page 209, last paragraph, discussion about potential d-excess product and potential reasons for disagreement with ECHAM: the authors should be more careful when discussing potential d-excess data! According to Fig. 9 the ECHAM d-excess value is within 5-15‰ (signal variation of less than 10‰). In order to detect this small signal the $\delta^{18}O$ data need to have a precision of almost 1‰! Already the uncertainty due to the apriori assumed relation between the isotopologues means a $\delta^{18}O$ uncertainty of 0.5‰ (see page 206, line 15). To that value the authors must add the uncertainty caused by the assumed NCEP apriori profile (an uncertainty estimation which they still need to make …). Furthermore, there is an uncertainty in δD …

In general I think the authors need to better take into account the uncertainties due to their apriori assumptions when discussing the differences between their products and the model data.

(9) Fig. 8, 9, 10: Do the measurements really introduce new information? We must remember that the retrieval uses a lot of apriori information and the variation as seen in the calculated δD and $\delta^{18}O$ might be already seen in the apriori data. The authors should test this: First, they should plot the δD and $\delta^{18}O$ data as calculated from the retrieved $H_2{}^{16}O$ according to Eqs (3) and (4). Second, they should investigate if the so-calculated δD and $\delta^{18}O$ data is really significantly different from the δD and $\delta^{18}O$ data as calculated from the retrieved $H_2{}^{16}O$, $H_2{}^{18}O$ and $HD^{16}O$. It might be that it is sufficient to retrieve $H_2{}^{16}O$. The authors should answer the question if the $H_2{}^{18}O$ and $HD^{16}O$ retrievals really add complementary information?

Minor remarks (typos):

(1) Page 196, line 26: evaporates -> evaporate
(2) Page 199 line 11: This reference is not correct here. Instead, the authors should put it at page 198, line 3, where they talk about IASI retrievals.
(3) Page 200, line 15: by THE TCCON
(4) Page 201, line 4: remove “yr”
(5) Line 5: taken UNDER different conditions
(6) Line 11: used BY THE TCCON
(7) Line 15: example of THE retrieved scaling factors of THE apriori