Response to Referee #1: Matthias Schneider; Dec 2018

Black: Referee's comments
Green: Author's reply

We would like to thank Matthias Schneider for his helpful comments and suggestions. We have taken all the comments into account. In our opinion, the revised has improved thanks to suggestions provided by both reviewers.

the manuscript addresses the following topics:

(1) it describes the retrieval of water vapour profile from ground-based FTIR measurements, (2) it compares the retrieval data with frost point hygrometer sonde data, (3) it assess the impact of different WV a priori data on the retrieval of water vapour, and (4) it assess the impact of different WV a priori data on the retrieval of other trace gases where water vapour is an important interfering species.

My general comments:

I find (4) is a nice and valuable demonstration of the importance for using actual WV profile data in order to avoid large uncertainties in the retrievals of other trace gases. The reason is that WV is very variable and not well capturing the variability results in large retrieval errors of the other species. However, this part of the paper could be further improved by inserting references on previous work where the interference error of WV has been calculated.

We appreciate this comment. It was valuable that the reviewer included references (in the specific comments) from previous work. We have included the references in the revised manuscript. Please see also our response in the specific comment provided below.

I think (1)-(3) need revisions. A constrained remote sensing data product (here x_r) means that a priori data (here x_a) has been updated with a measurement. The product (x_r) strongly depends on the a priori data (x_a). In particularly if x_a is variable on small scales (like for WV) the variability in x_r will, to a large extent, reflect the variability of the prescribed x_a. Instead of assessing the quality of x_r the authors should assess how the remote sensing measurement can improve the assumed a priori state of the atmosphere, i.e. the authors should validate x_r-x_a by comparing it to A(x_s-x_a), where x_s is the FPH reference.

This point is well taken and along with suggestions from reviewer #2. In the revised manuscript we have included comparison of retrieved WV and sonde FPH using the formalisms by Rodgers and Connor (2003). Figures 5 and 6 include smoothed FPH profiles using equation 4 in Rodgers and Connor (2003), instead of showing them in the supplemental material (like the initial version). Additionally, we have included in the main text, results of comparisons between FTIR retrievals for both un-smoothed & smoothed FPH. We kindly refer the reviewer to the revised manuscript for additional/modified text and figures. In particular, table 3 summarizes the findings of both comparisons. Furthermore, in the revised section 4.3 we added a short description regarding the value of x_r-x_a. Please see our response in the specific comments below.

Furthermore, when using an a priori data that already captures most of the variability, the solution state should be more constrained (the S_a matrix should have much smaller entries) than when using an x_a that captures only few variability. However, judging from Sect. 3 it seems that the authors use a single S_a for constraining the different retrievals.

This has been addressed in the specific comment below.

Specific comments:

I have inserted my ideas/suggestions in the attached pdf version of the manuscript.

Best regards.

Comments provided by the referee are copied from the pdf and shown below in back.

Summary of Comments on amt-2018-283_MS.pdf

Page: 2
Number: 1 Author: pa5682 Subject: Cross-Out Date: 12/3/2018 8:01:36 PM

Accepted, text has been removed.

Number: 2 Author: pa5682 Subject: Inserted Text Date: 12/3/2018 7:55:01 PM
uses

Accepted.

Number: 3 Author: pa5682 Subject: Inserted Text Date: 12/3/2018 10:25:15 PM
/FTIR spectra measured at 12 different sites

Included with minor edits.

Number: 4 Author: pa5682 Subject: Inserted Text Date: 12/3/2018 10:36:31 PM
for generating a long-term data set of global representativeness of tropospheric water vapour profiles with a DOFS of almost 2.8 and of about 1.6 for the ratio between the most abundant isotopologue H216O and the heavy isotopologue HD16O.

Included with minor edits.

Number: 5 Author: pa5682 Subject: Inserted Text Date: 12/3/2018 8:03:40 PM
Comparisons of FTIR and operational radiosondes have been used to validate optimized WV profile retrieval strategies (e.g. Schneider et al. 2006; Schneider and Hase, 2009; Schneider et al., 2016).

Included with minor edits.

The complete paragraph now is:

MUSICA (MUlti-platform remote Sensing of Isotopologues for investigating the Cycle of Atmospheric water) is a project within the NDACC/FTIR using standard spectra from a subset of NDACC sites in order to generate a long-term data set of tropospheric water vapor profiles with degrees of freedom (DOF) of about 2.8 and of about 1.6 for the ratio between the most abundant isotopologue $H_2{}^{16}O$ and the heavy isotopologue (Schneider:2012, 2016, Barthlott, et al., 2017). Comparisons of FTIR and operational radiosondes have been used to validate optimized WV profile retrieval strategies, (Schneider et al., 2006; Schneider and Hase, 2009). Vogelmann et al. (2015) studied the spatial-temporal variability of WV in the free troposphere (Zugspitze, Germany) by exploiting the geometry of measurements of differential absorption lidar (DIAL) and FTIR. In particular, they assessed the variability in short scales, i.e., few kilometers and minutes."

Number: 6 Author: pa5682 Subject: Inserted Text Date: 12/3/2018 10:37:43 PM
made at two different sites, that have so far not been considered within MUSICA. We use spectral microwindows that are not identical to those of
MUSICA (Barthlott et al., 2017, Fig. 1 therein) and perform the inversion on a linear scale (instead of a logaritmic scale used by MUSICA

Thanks for pointing this out. Rather than in the introduction these details have been included in Sect 3 (Retrieval of water vapor from FTIR). The following sentence is now in Sect 3:

"We use spectral micro-windows that are not identical to those of current MUSICA version (Barthlott et al., 2017) and perform the inversion on a linear scale (instead of a logarithmic scale used by MUSICA)."

Page: 5
Number: 1 Author: pa5682 Subject: Highlight Date: 12/7/2018 7:19:46 PM
For constraining the authors use the same S_a^-1 for the different a priori from Section 4.3? If yes, the solution state will be much looser constraint for the daily varying a priori than for the monthly varying a priori, i.e the two retrievals are difficult to be compared.

In principle, we agree that Sa might need an adjustment depending on the a priori, especially for gases with less variability. The variability of water vapor can be large and not necessarily the Sa of the daily a priori is always much looser than the monthly profile. There are cases where even the daily a priori is distant from the "real" or retrieved WV but the monthly a priori is better. Optimizing a Sa for one day might not necessarily be best for another day. Furthermore, there are several reasons why we use a single Sa: (1) this work does not aim to optimize retrieval parameters but rather use a common retrieval approach that could be applicable to more sites; (2) the standard Sa used here has been optimized in all cases in order to obtain similar information content; (3) three out of four a priori are similar and we expect similar Sa and changing Sa would result in a more complex comparison.

We value this comment and in the revised manuscript we include this modified text (please note that it was modified also following the suggestion of reviewer #2:

"*The Sa matrix is specified at each layer as a fraction of the a priori profile, which allows for a linear scaled retrieval. We adopted a maximum variability of 50 % in the diagonal covariance and exponentially decreasing by altitude. In order to prevent sporadic vertical profile oscillations, we include a Gaussian correlation length of 25 km in the off-diagonal elements of Sa. This Sa has been optimized in order to obtain similar information content for all a priori presented in section 4.3, a requirement for efficient processing of decades of NDACC spectra.*"

In addition, in the conclusions we mentioned that further optimization of the a priori covariance matrix might be needed in future research. The paragraph reads as:

"Further research would explore the additional WV absorption features in order to improve the information content, e.g., micro-windows employed in the latest MUSICA version. Also, as we show, the ERA-I WV profiles yield lower biases, hence we would construct a priori covariance matrices for these that maximize accuracy and vertical structure."

Page: 6

Number: 1 Author: pa5682 Subject: Highlight Date: 12/7/2018 6:24:45 PM
It is important to describe here the remote sensing measurement as an update of the a priori information, i.e. the actual measurement is x_r-x_a not x_r! The authors should explain how the a priori affect the retrieval results: x_r = A(x-x_a)+x_a+Dx, where Dx are retrieval errors. Because A is not an identity matrix x_r will always significantly depend on x_a.

We include a description of the effect of the apriori in Section 4.3:

"The optimal estimation method is influenced by the a priori profile because it may bias the solution of equation 1. Since WV is highly variable, even in time scale of hours, using the most accurate a priori might improve the retrieval results. In general, the retrieval of WV can be seen as an update of the a priori information."

The authors use variable a apriori data (see Sect. 4.3) and the variability seen in the retrieved vertical profile reflects to large extent the variability prescribed by the a priori data. Unfortunately this is not correctly considered in Sect 4 of the paper. Because the authors work with a variable a priori they should evaluate the signals in x_r-x_a=A(x-x_a), because this is the mesured signal not x_r=A(x-x_a)+x_a!. Furthermore, the authors assume that if x_s can be used as a reference for the retrieved profile x_r; howrever, actually x_s is highly resolved and absolutely calibrated reference, i.e. it is a reference for the real atmospheric profile x. So correcty the authors should compare x_r-x_a with A(x_s-x_a) in order to validate the remote sensing measurement.

In the revised section 4.3 we added a short description regarding the value of x_r-x_a to evaluate signal of the measurements:

"Additionally, the difference between WV retrievals and a priori profiles (x_r-x_a) provides further evidence in the measured signal and to some extent the variability prescribed by the a priori (Rodgers and Connor, 2003). For example, this difference is about 11 +/- 38 % using ERA-6 while for WACCM is about 29 +/- 32 % for the first layer. As we expected, from these observations it can be seen that the WACCM climatology as a priori results in greater deviations compared to ERA-6."

As pointed out before for the comparison we follow the formalism of Rodgers and Connor (2003) in addition to the un-smoothed comparisons to assess vertical gradients and avoid averaging kernels limitations.

Page: 12
Number: 1 Author: pa5682 Subject: Highlight Date: 12/4/2018 2:10:17 PM
The retrievad data x_r are almost not sensitive to atmospheric variations above 10km, so I suggest not showing layers above 10km.

We have removed the last two layers and text has been modified accordingly.

Page: 13
Number: 1 Author: pa5682 Subject: Highlight Date: 12/4/2018 2:14:12 PM
monthly varying a apriori is used, please specify?

"a 40 year simulation (1980-2020) of the WACCM mean profiles"

Number: 2 Author: pa5682 Subject: Highlight Date: 12/4/2018 2:14:56 PM
daily varying a priroi?

"daily varying (ERA-d)"

Number: 3 Author: pa5682 Subject: Highlight Date: 12/4/2018 2:15:31 PM
6 hourly varying a priori profile?

"6 hourly varying WV vertical profiles (00, 06, 12, and 18 UTC) obtained from ERA-I (ERA-6)"

Number: 4 Author: pa5682 Subject: Highlight Date: 12/4/2018 2:16:28 PM
daily varying a priori profile

"daily varying NCEP/NCAR (NCEP-d) reanalysis WV profiles"

Number: 5 Author: pa5682 Subject: Highlight Date: 12/4/2018 2:28:19 PM
If x_s is the reference x_r-x_s=A*(x_s-x_a)-(x_s-x_a)+Dx=(A-I)*(x_s-x_a)+Dx
Dx are the retrieval errors

This is correct but we do not have anything to add.

Page: 14
Number: 1 Author: pa5682 Subject: Highlight Date: 12/4/2018 2:36:40 PM
x_r-x_s=(I-A)*(x_a-x_s)+Dx, i.e. it depends on the retrieval errors Dx and on (x_a-x_s). Because a daily or even 6 hourly varying x_a better captures the actual variability of atmospheric WV, using x_a from ERA-d and ERA-6 (instead of monthly climatologies) better captures the variability as given in x_s, i.e. x_r-x_s shows a particular small scatter. This is no surprise.

In general, this might be true, but in this work, we present a quantitative assessment of the different a priori, even for daily or 6 hourly.

Page: 15
Number: 1 Author: pa5682 Subject: Highlight Date: 12/3/2018 10:59:53 PM
see comment on Table 2

ok

Number: 2 Author: pa5682 Subject: Highlight Date: 12/3/2018 11:39:37 PM
Here retrieval data generated by using varying a priori data are compared to the sonde measurements. This does not allow robust conclusions on the quality of the FTIR measurements. Actually there will be a very good agreement already by comparing the varying a priori with the sonde measurement (i.e. without any information from the FTIR measurement).
What you need to compare and evaluate is the difference with respect to the apriori! So you have to calculate x_r-x_a and correlate it to A*(x_s- x_a).

In the revise table we have added the comparison using the formalisms by Rodgers and Connor (2003), i.e., smoothing the FPH profiles using the water vapor averaging kernels. Note that results using "un-smoothed" are also shown. The limitations of the averaging kernels are seen clearly in this table.

Page: 16
Number: 1 Author: pa5682 Subject: Highlight Date: 12/5/2018 3:03:57 PM
There is some work:
The impact of interferences from WV on the retrieval of CO has been estimated by Sussmann and Borsdorff, 2007 (doi:10.5194/ acp-7-3537-2007), on the retrieval of O3 by García et al. 2014 (doi:10.5194/amt-7-3071-2014) and on the retrieval of CH4 by Sepúlveda et al., 2014 (doi:10.5194/amt-7-2337-2014).

Thanks for providing the references of previous works. The text in the revised manuscript has been edited to include the references provided. We note that García et al. (2014) and Sepúlveda et al. (2014) retrieved water vapor in a first step to minimize errors in the retrieval of O_3, and CH_4, respectively. Sussmann and Borsdorff. (2007 quantified the impact of water vapor in the retrieval of CO and further apply a retrieval strategy to remove interference errors. Still, the effect of using co-located and highly-resolved WV are missing in the literature.

Page: 17

Number: 1 Author: pa5682 Subject: Highlight Date: 12/7/2018 6:45:22 PM
The strategy is sufficient to avoid WV interferences in the retrievals of other trace gases and the obtained WV profiles are of a reasonable quality. However, using retrievals with more WV lines, and retrievals on log scale (tropospheric water vapour is log-normally distributed) should theoretically provide better results. Actually the MUSICA WV data show higher DOF and agreement with radiosonde also within 10-20%

The above suggestion has been included and reads as follow:

"This example suggests that the current retrieval strategy of WV is suitable to avoid WV interference in the retrievals of other trace gases."

In addition, in the conclusions we included the following:

"Further research would explore the additional WV absorption features in order to improve the information content, e.g., micro-windows employed in the latest MUSICA version. Also, as we show, the ERA-I WV profiles yield lower biases, hence we would construct a priori covariance matrices for these that maximize accuracy and vertical structure."