Atmos. Meas. Tech. Discuss.,
doi:10.5194/amt-2019-240-AC2, 2019

Atmospheric Measurement Techniques Discussions

Interactive comment on "First data set of H_2O/HDO columns from TROPOMI" *by* Andreas Schneider et al.

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Received and published: 24 October 2019

The manuscript "First data set of H2O/HDO columns from TROPOMI" by Schneider et al provides a first glimpse into the excellent data quality of novel isotopologue measurements from the TROPOMI instrument. As a "first data" paper, it provides a well rounded overview of validation and a few examples of HDO/H_2O δD distributions. Overall, this paper is well suited for AMT and should be published after minor revisions. I also apologize for the late review. Please find some comments (High level first, then detailed aspects) below:

The authors would like to thank for the positive and constructive review. In the following, all individual comments are quoted in italics and our response is given below.

High Level comments

- *I would really like to see at least one spectral fit in a first data paper but am missing a discussion on fit quality, spectral residuals and the like in this manuscript. Please provide a figure showing typical fits, potentially systematic residuals and locations of HDO and H_2O lines (e. g. plot Jacobians and spectral fits + residuals, a few examples are enough but this being a "first data" paper, I consider this a must).*

  Plots of a TROPOMI radiance measurement with spectral fit, the corresponding residual, and absorption of H_2O, HDO and CH_4 have been added. Moreover, χ^2 was added to all time series and statistics plots.

  In this context, the time series has been extended with new TCCON measurements that have newly become available, which slightly changes the validation results.

- *The averaging kernels for H_2O could be an issue for some of the data analysis, especially if parts of the lower column might be blocked by fractional cloud cover. I understand that the authors strictly filter data to alleviate this problem but I am also wondering whether you can make the averaging kernel more uniform for H_2O. There might be a few options. A profile fit could help achieving this, even if the degrees of freedom won't be necessarily high (did you ever try)? You might also try to block out the strongest H_2O lines in the retrieval, which might help (the weaker the lines, the more uniform the averaging kernels). In the long run, this could/should be a focus for further retrieval work as it would allow you to relax filter criteria. However, I realize that this is a bigger endeavor and will require more work in potential future papers.*

  Setting up a profile retrieval would need a different algorithm and is out of the scope of this paper. Moreover, due to the spectral resolution and the signal-to-

noise ratio of the measurement we believe that the information content is not more than one degree of freedom for HDO.

We tried a few different spectral windows, for instance with weaker H_2O lines, but the averaging kernel of H_2O changed only little. Furthermore, in the spectral range of the SWIR channel without very strong H_2O lines there are only very weak HDO lines so that no useful retrieval of HDO is possible there.

- *In many plots, you always discuss and show "biases", which are additive in nature. However, your analysis uses scaling factors, which are multiplicative. Multiplicative biases are natural, as line strengths in databases can be wrong but it also means that additive biases depend on the amount itself. I would change all bias discussions/plots into relative terms (% bias is basically multiplicative). For fits, provide slope and intercept (e. g. in Figure 5).*

  In the revised version, relative biases are shown additionally to the absolute biases.

  We have added a fit to the correlation plots in Figure 5 (now Figure 6) and give the respective slope and intercept.

- *I am missing a Rayleigh plot to be honest, maybe pick a few regions and plot H_2O column amount vs delta-D? Would be good just to show the general dependence. Could also be plotted along a typical transect.*

  We have added a Rayleigh plot for the case study of the blocking anticyclone in Section 5 in form of a histogram with contours for the cumulative density together with a Rayleigh fractionation line and three mixing lines, as well as a discussion of it in the text.

Detailed minor comments

- *Abstract: Maybe start with a more general scientific scope sentence in the very beginning*

  We have added the following sentence:

  Global measurements of atmospheric water vapour isotopologues aid to better understand the hydrological cycle and improve global circulation models.

- *around line 45: make clear that thermal and SW satellites have very different sensitivities.*

  We have added the following two sentences:

  The sensitivity of instruments observing in the thermal infrared (IMG, TES, MIPAS, IASI, AIRS) is very different from that of instruments measuring in the shortwave infrared like SCIAMACHY and GOSAT. While the former are mainly sensitive in the stratosphere and free troposphere, the latter have good sensitivity in the lower troposphere including the boundary layer.

- *line 57: data "are" (data is plural)*

  Not sure what you are referring to. In the sentence in line 57, "the comparison between both data sets is performed in Section 4", the "is" refers to "comparison".

- *line 65 "with an order 1 Lambertian albedo", be more specific (I know what you mean). Also, is order 1 enough? Did you try higher orders? If not, why not?*

  We have rephrased that as "together with a Lambertian surface albedo in the form of an order 1 Legendre polynomial".

  We have tried retrievals with different orders. With order 0 the residual is tilted. For orders higher than 1, the difference to order 1 is not so large, and it is beneficial not to waste too many degrees of freedom here.

- *Line 69: Do I see it correctly that your delta-D prior profile is 0?*

  Although δD is not explicitly retrieved, the prior profiles of H_2O and HDO result in an implicit prior of δD of 0 ‰. In the manuscript we have added the following sentence:

  That implicitly corresponds to a prior of δD of 0 ‰.

- *Line 77: Diffraction effects are not really the biggest problem I would say (generally more scattering at higher angles, longer light-paths, etc. . .)*

  We have rephrased this sentence as follows:

  Furthermore, scenes with solar zenith angle greater than 75° are discarded because they are prone to errors due to more scattering and diffraction effects which are not covered well by the forward model and due to typically low radiances meaning low signal-to-noise ratio.

- *Figure 1: Plot with pressure on Y-axis would be more representative.*

  The averaging kernel is now plotted in pressure coordinates with a logarithmic pressure axis.

- *Figure 2: Again, bias is misleading here. Express it in %, not absolute terms. How about intercept issues?*

  We have added the relative bias. Not sure what exactly you mean with "intercept issues". We have added a linear fit with slope and intercept in Figure 3a (now Figure 4a) and the confidence interval computed with the bootstrap method. The original fit is included in the confidence interval, thus there are no significant intercept issues. The manuscript has been updated accordingly.

- *Line 126: molcec*

  This typo has been corrected.

- *Line 135: "is plain": What do you mean?*

  We have rephrased this to "is clearly visible".

- *Figure 6: show relative biases, not absolute*

  We additionally show relative biases in the revised version. To this end, we have split the figure in two, one for the statistics and one for the biases.

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