

Atmos. Meas. Tech. Discuss., author comment AC2
<https://doi.org/10.5194/amt-2021-141-AC2>, 2021
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Reply on RC2

Andreas Schneider et al.

Author comment on "Retrieving H₂O/HDO columns over cloudy and clear-sky scenes from the Tropospheric Monitoring Instrument (TROPOMI)" by Andreas Schneider et al., Atmos. Meas. Tech. Discuss., <https://doi.org/10.5194/amt-2021-141-AC2>, 2021

The manuscript by Schneider et al is a valuable contribution towards the application of global HDO/H₂O data for scientific interpretation. While the paper is in general well written, I have a few points/concerns that require consideration.

Thank you for your positive judgement of our contribution and for your review. In the following, all individual comments are quoted in italics and our response is given below.

Major points:

Retrieval:

In table 1, you list a reduced chi² filter of <150. Is this really the reduced chi²? If yes, 150 as a cutoff appears extremely high, i.e. you are not fitting the spectra properly. Given your regularizations, I would really like to see typical residuals of your spectral fits.

We have added a plot of a residual of a scene over the Sahara with high reduced χ^2 (around 130). The fit is good and the residual looks normal. The very high signal at the bright scene amplifies errors due to inaccuracies in the spectroscopy and thus results in high reduced χ^2 . That could in principle be eliminated by a different normalization.

Surface albedo prior: I am somewhat concerned about your choice of a surface albedo prior, using an annual average. This could create seasonal biases in your retrieval, depending on how strongly you regularize the retrieval. Some more details would be good to show that this is NOT the case. Also, what do you assume as the spectral dependence of your surface albedo in the fitting window? Varying snow cover and vegetation growth can cause large seasonal cycles in albedo, so using an annual average as prior seems to be not a great choice (MODIS provides more than enough data to get monthly priors).

We assume a linear spectral dependence of surface albedo in the retrieval window. The spectral slope is also derived in the inversion but not regularized. The regularization of the albedo at the centre of the spectral window is weak to give the algorithm enough freedom to adapt it to the actual situation.

We have tested potential seasonal effects for scenes collocated to TCCON measurements by performing retrievals using a priori surface albedo from the (D)LER data product from the S5P+ Innovation Aerosol Optical Depth (AOD) and Bidirectional Reflectance

Distribution Function (BRDF) project (Tilstra, 2021), which features monthly values. The results are very similar to those with the one-year average a priori, although the changed albedo prior results in slightly less convergences.

Averaging kernels and profile scaling: It seems you are using a profile scaling approach, which might explain the somewhat counter-intuitive averaging kernels shown in Figure 10. As you only scale the profile: How do you compute (and provide) the column averaging kernels with your retrievals? It seems the data would be rather unusable without the kernels. Also, why did you choose not to fit the profile? While your DOF might not be $\gg 1$, it would help not getting extreme values in your column kernel. In Figure 10, I would also suggest to plot the kernels with pressure as y axis. Given the scale height of H₂O is low, the higher altitudes are rather unimportant for SWIR HDO/H₂O retrievals.

The data product provides column averaging kernels for each individual TROPOMI ground pixel. These are computed as described by Borsdorff et al. (2014) who showed that a total column averaging kernel can also be computed analytically for a profile scaling retrieval. We agree that providing the column average kernel to the user is important.

The data do not contain enough information to do a profile retrieval (DOF ≈ 1).

Averaging kernel plots are now shown with pressure as y axis.

Science:

In your example cases, it would be good to really point out what could be learned from delta-D rather than just H₂O alone. At the moment, this is unclear. More Rayleigh plots (e.g. a density plot of your global dataset) would be very helpful.

Thank you for this important comment, in particular the idea of showing an additional (H₂O, δD) plot for the global dataset to highlight the additional use of δD . We have added a new figure depicting the (H₂O, δD) distributions for September 2018 over tropical lands and ocean and shortly discuss in Section 5.1 examples of what can be learned from the additional use of the δD data from the scattering retrieval. In Section 5.2, we have pointed out the new insight from δD by adding the following sentence at L391:

“Vertical mixing between the boundary layer and the free troposphere, such as during the moistening of the cold sector is one key process for which isotopes could provide additional information compared to total column H₂O only.”

However, it is not the role of this technical study to highlight the benefit of δD for the study of different moist atmospheric processes, for this we refer to targetted scientific papers such as Risi et al. (2021), Thurnherr et al. (2021), Aemisegger et al. (2021) and many more.

Small issues:

Line 40: is notified?? I think I know what you mean but it won't be clear

This sentence is rephrased as follows: “Any loss of sensitivity to the partial column below the cloud is reflected in the column averaging kernel.”

Line 61: Absorption cross section (not scattering)

Changed.

Line 80: Interferences and biases: Would be good to show spectral fits to maybe provide

some more evidence to the gut feelings expressed here

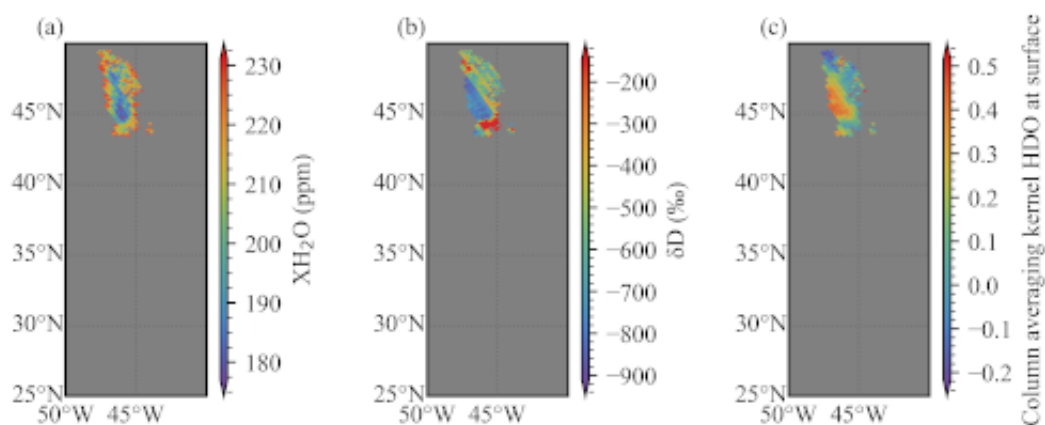
We add a plot of a spectral fit.

Line 134: just saying "unit vector" is fine

Actually, it is not a unit vector (1, 0, 0, ...) but a vector with ones in each place (1, 1, 1, ...). We have clarified the sentence by rephrasing it to "a vector with ones in all places".

Figure 18: In the left panel, there seems to be a high density region with very low H₂O crossing over all possible delta-D values. This seems somewhat unphysical, do you have an explanation for that? Could you plot the locations of this weird "vertical stripe" of data in the density plot?

We have found a bug in the original plot script for the Rayleigh plot that resulted in the use of wrong filter parameters (thresholds). That has been corrected in the new version. However, there is still a stripe in the new version of the plot. The requested plot with the location of the low humidity data is shown below. Currently it is unclear whether the stripe is an artefact. The issue will be further investigated.



TROPOMI single overpass results of XH₂O (a), δD (b) and the column averaging kernel at the surface layer (c) for H₂O columns below $5 \times 10^{21} \text{cm}^{-2}$ on 19 January 2020

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