

Comment on amt-2021-32

Anonymous Referee #2

Referee comment on "Ozone profile retrieval from nadir TROPOMI measurements in the UV range" by Nora Mettig et al., Atmos. Meas. Tech. Discuss.,
<https://doi.org/10.5194/amt-2021-32-RC3>, 2021

This paper presents a new TROPOMI ozone profile retrieval from UV (UV-1 and UV-2) measurements using the Tikhonov regularization based TOPAS algorithm. A sensitivity study is presented to show the retrieval quality from synthetic data. Systematic biases in TROPOMI data are shown by comparing simulation using MLS+MERRA-2 ozone profiles with observation, and soft calibration is derived and applied to the retrievals. The retrievals are validated with ozonesonde and lidar measurements as well as MLS, and OMPS satellite measurements. Examples of global distribution of ozone at different altitude ranges are shown. The scope of this study is well suited for AMT. This paper is generally well organized and methodology is generally good. However, some of the important retrieval details are not described and some places require clarification. Overall, I think that this paper can be published after addressing the specific comments below.

Specific comments:

- L38, SAGE-III on ISS was launched in 2017, not 2006. Suggest changing to "launched in 2001 on Meteor-3M and in 2017 on ISS"
- L77, I think that it should be "in-flight analyses"
- L81-84, it would be useful to describe a little more about ozone profile retrievals by Zhao here in addition to the spectral range: for example, using the optimal estimation method, also derive and apply soft calibration. Band 3 is used due to larger systematic radiance differences in band 1 and larger fitting residuals in band 2, and larger biases in total ozone and ozone profile with relative to other correlative measurements.
- L113, should the spatial resolution of retrievals at nadir be $28.8 \times 45 \text{ km}^2$ due to coadding of 8 UV2 across-the-track and 8 pixels along the track?
- L130, according to how SNR is calculated in the L1b (mostly Poisson noise), I think that

the binned error should be $1/\text{SQRT}(n) * \text{SUM}(\text{SNR}_i)$. If $n=1$, according to your equation, $\text{SNR}_{\text{binned}} = 1/\text{SQRT}(2) * \text{SNR}$ rather than SNR.

- L150, please check the reference as Flynn et al. (2014) does not talk about LP retrievals. A better reference the LP measurements may be Jaross et al. (2014): <https://agupubs.onlinelibrary.wiley.com/doi/full/10.1002/2013JD020482>
- L167, for the temporal collocation criterion, it says "24 hours time differences", as it is a fixed time difference here, suggest changing to "within 24 hours" or "24 hours maximum time differences". Also, I guess most of the time differences are within 12 hours. You may tighten this criterion.
- L184, the full name of TOPAS has been mentioned earlier in the introduction, so you do not need to mention here again.
- Table 1 is not referenced in the text. You may mention Table 1 at the beginning of Sect. 3.2 before describing the retrieval in more details.
- L215, you may add "base on LUT" after "A polarization correction" and add " and will be described later in this section"
- L216, based on the text below, offset is also fitted. So you add it to this sentence. Why is a 1st order polynomial subtracted? L256 also does not mention why and what kind of 1st order polynomial is subtracted. Is the 1st order polynomial pre-determined?
- In table 1, it is not clear about how and why Tikhonov 0th order parameter of 11.11 is set. According to equation (4), the 0th Tikhonov term is just Sa^{-1} .
- L255, what do you mean "represented by the inverse solar spectrum"? Are you fitting a scaling factor to the solar spectrum? Please clarify it.
- L264, you may change to "in generally good agreement on altitude average" as the actual variance changes a lot.
- L268, the gamma value is fixed to 0.007 for all the retrievals here. In the Tikhonov method, the regularization parameter (i.e., gamma here) is often determined dynamically, for example, using the L-curve method. Have you tried to derive it dynamically?
- L272-273, has the noise in the solar irradiance been included in the calculation of SNR?
- L277-278, it is not clear about how "no cross-talk between these two parameters is considered while both are retrieved in one iterative step. I guess that the covariance terms in Sa are 0 between ozone and surface albedo parameters. Do you also set the Jacobians for effective surface albedo to 0 below 310 nm?
- In Fig. 2, do the green curves on middle and bottom panels show the mean differences between retrievals and convolved true profiles? Or do they show the differences between the mean retrievals (orange with circles) and convolved true profiles? It is not clear from the figure caption.
- In Fig. 3 caption, the total retrieval error (black) is not seen and also not shown on the legend of panel (e). Should the layer legends on Fig. 3c be 0.5, 5.5, ... 59.5 km. From the text, the retrievals are done at 60 layers, but on Figs. 2 and 3, the results are plotted at 61 levels from 0 to 60 km. Please clarify this.
- L360, based on the definition of vertical resolution as the inverted main diagonal (i.e., layer degree of freedom for signal), the vertical resolution becomes smaller if the retrieval is done at a coarse grid (e.g., every 5 km). Does this definition require the retrieval to be done at every 1 km or require the normalization to layer thickness?
- L365 and Fig. 3e, the noise errors and standard deviations of retrieval results seem to be too small to be true especially in the lower stratosphere and troposphere. Please check them. What are the binned SNRs at different wavelengths for this specific spectrum?
- L375-376, it cannot be seen from Fig. 4 that the vertical resolution improves for the bottom layer as the values become much larger for the bottom layer.
- L383-385, based on Fig. 4, the sentence "At larger SZA, ... with increasing VA below 17 km" is true for relative azimuthal angle of 180, but opposite for relative azimuthal angle of 0. Can you please explain why the vertical resolution depends so greatly on VA for large SZA and the dependence is on the opposite? The troposphere becomes invisible at SZA of 85 except for VZA 50/54 and relative azimuthal angle of 0, right? Why the

vertical resolution significantly increases for VZ 50/54? Is this real or due to some kind of anomaly in the averaging kernels?

- L392-394, how and how much do the additional independent variables generally change the DOF?
- L466-499, the first sentence say "the increased vertical resolution found in this altitude range, see Fig. 4." But according to Fig. 4., the values at few bottom layers increase (compared to 3-5 km?) and thus the vertical resolution become worse. Also for some of the larger SZAs or high latitude, the vertical resolution decreases in this altitude range and the retrieval sensitivity is very limited in 0-5 km. So I think that this statement is not accurate. Also to show the retrieval improvement over the a priori, I think that it is equally important to show the improvement of standard deviation of the differences. So at what altitude/latitude ranges are the standard deviations of the differences between retrievals and ozonesonde better than those between a priori and ozonesonde?
- L470-476, it is also useful to discuss about the slope and whether the retrievals improve over the a priori.
- Figure 9 legend, "num. sondes" should be "num. Lidar"
- L496-497, it is likely due to reduce retrieval sensitivity for these altitudes? What are the precision for lidar measurements at these altitude ranges.
- L506, are you getting a priori ozone between scene pressure and surface pressure? Or do you retrieve ozone only above scene pressure?
- L503-506, it is worth to add that the 0-8 km sub-columns show high wave one pattern in the tropics, with high ozone in the South Atlantic and low ozone in the tropics, and generally higher ozone at mid-latitudes as these features are generally consistent with the tropospheric ozone distribution.
- L510 and L534, I suggest changing to "no vertical information" as there is still useful information for the sub-columns.
- L562-563, this seems to suggest that the TOPAS total ozone at high latitudes is less accurate compared to WFDOAS total ozone. I think that WFDOAS retrievals might be more sensitive to a priori ozone as no vertical ozone information is retrieved.

Technical comments:

- Title: Some words (not prep. or adv.) are not capitalized: nadir, measurements, range. You may remove "nadir" as TROPOMI is a nadir-viewing only instrument.
- In abstract, it might be useful to show the unabbreviated name of "TOPAS" algorithm at its first occurrence.
- In abstract, you may show full name of "TROPOMI" as "Tropospheric Monitoring Instrument (TROPOMI)", "MLS" as "Microwave Limb Sounder (MLS) on the Aura satellite", and of "OMPS-LP" as "Ozone Mapping and Profiler Suite Limb Profiler (OMPS-LP)" at their first occurrences
- L51, change to "higher" and use subscript for 3 in O₃
- In equation (6), S_R should be S_r for consistency.
- L220, there is an extra "." after "a priori"
- L225, miss an "." Before "The effective"
- L228, good to specify the unabbreviated names of OCRA and ROCINN.
- L271, "y" in "Sy" should be in subscript
- Figure 2 caption, add 's' to "difference"
- 10 L328, change to "independent of"
- L422, there is an extra ")"
- L427, suggest changing to "and tends to be negative" and "A closer look at" or "A closer look into"

- L540, change to "i.e."