Atmospheric Measurement Techniques Discussions

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RC1: Comment on amt-2021-201

Anonymous Referee #1

Referee comment on "Retrieval of tropospheric aerosol, NO2 and HCHO vertical profiles from MAX-DOAS observations over Thessaloniki, Greece: Intercomparison and validation of two inversion algorithms" by Dimitris Karagkiozidis et al., Atmos. Meas. Tech. Discuss., https://doi.org/10.5194/amt-2021-201-RC1, 2021

General comments

Karagkiozidis et al. present a comprehensive comparison and validation study of two MAX-DOAS profiling algorithms. The algorithms retrieve trace gas and aerosol profiles from MAX-DOAS observations over Thessaloniki, Greece.
The manuscript is well written, the analyses have been performed thoroughly and the conclusions are interesting.

However, while reading this document, I was wondering, what is the aim of this study? From the title, I expected a characterization of the temporal and spatial distribution of NO2, HCHO and aerosols over Thessaloniki. But the authors focused mainly on the comparison and validation of two profiling algorithms. Algorithms which have already been validated in other studies! In my viewpoint, the authors should change the manuscript slightly in order to go more in the direction of either a pure algorithm validation/verification paper or a characterization paper of Thessaloniki's trace gas/aerosol distribution.
If the authors decide for case 1, I would expect a detailed comparison of vertical profiles. If validation is not possible due to sparse measurements of ancillary instruments, please add a comparison of temporal/spatial mean profiles of both algorithms. I was also wondering if MAPA retrieves concentrations in higher altitudes compared to MMF? On the other hand, MMF does not retrieve small VCD's even though the correlation with in situ data is high. Does the a priori SH of 1km leads to this constrain? If the manuscript is modified based on these suggestions, please change the title accordingly.
In case the authors decide for a characterization paper of the tropospheric composition over Thessaloniki, I would expect a discussion of weekday to weekend variations. I would also expect diurnal variation plots. Furthermore, in this case, the analysis of HCHO is insufficient. Even
though validation is not possible we learn nothing about the spatial distribution of HCHO from your study. You neither show HCHO profiles nor do you talk about possible sources (for all species).
In both cases, I would love to see some contour plots of seasonal mean profiles for all species.

Please also add the following points:

1. Even though the applied flags have been applied elsewhere, please add a table of flags for each algorithm in the appendix. I guess that
flagging thresholds might differ for UV and vis?
2. What is the conclusion of your flagging scheme discussion? I would consider your results as unclear. Maybe there is no clear conclusion to be made?
3. Please add a short discussion of NO_2 retrieved in the UV. You have mentioned that HCHO and aerosols in the UV might be negatively affected by increased spectral noise. Is there a similar conclusion for UV NO_2?
4. Please add a short discussion of possible issues of your aerosol retrieval due to the inaccurate Henyey-Greenstein phase function at the proper sections in your manuscript.
5. If I understand the authors correctly, the instrument measures in an altitude of 80m. How is this "elevated" position treated by the algorithms? What is the meaning of the lowermost retrieval grid point in this context?

Specific comments

P2, L43: "can lead to or") can lead to ... or deteriorate ...
P3, L81 - L84: You mention that the data is also analyzed regularly within the FRM4DOAS project. Please name the specific differences in retrieval settings between your study and the regularly submitted data and the reason for specific changes of settings. It would also be interesting to compare FRM4DOAS data with your new settings.
Fig. 2: Please add other instruments if not measured at the same location (e.g. in situ).
P10, L211: "by assuming a correlation length") "by assuming a Gaussian function with correlation length of...". Note that a correlation length of 50m was used in the cited publication!
P10, L224: What is the lowermost retrieval altitude for each algorithm? Surface values were extrapolated?
P12, L285: Why did you use hourly mean values? You could also average all in situ values for the corresponding MAX-DOAS elevation scan cycles.
P13, L288 - L292: I don't understand your reasoning here. I guess that tracffic emissions contribute strongly to the MAX-DOAS signal but then an in situ site should not be a background site. How far away is the next site in viewing direction of the telescope?
P13, L304: 5° is already quite small, especially when using Henyey-Greenstein. Have you tried different values? I would expect that 10° improves data quality significantly but might decrease the number of data points (maybe too much?).
P13, L308-L309: I am wondering how negative columns can make it through any flagging step? Also 8.5% is a really large fraction of invalid profiles. Is there any reason known why MAPA produces so many unrealistic profiles?
P14, Table 3: When looking at the HCHO fraction (also aerosols in UV) of valid profiles for MAPA, I am really worried about the general performance of MAPA in the UV. Is there any particular reason for this bad performance? There was already a BIAS found for MAPA's
HCHO results in Tirpitz et al. 2021 so I don't think that noisy data can explain everything!
P15, Figure 5: For reach row, MAPA shows values close to zero, except for NO2. I am not sure if it is a good thing, that MMF doesn't show small values at all or that MAPA cannot find them only for NO_2. Could you please say something about that? And again, I would be interested in MAPAS flagging thresholds and if they differ in the visible and UV spectral range.
P15, Figure 6: I think this figure tells us that MMF has a positiv Bias for low elevation angles (reddish dots more often over black line) which would also explain why we don't see small values in Fig. 5 for MMF. It seems that the algorithm has problems in retrieving accurate profiles
for small dSCD, especially in the UV. This could be explained by more noise but the MAPA results seem to be unaffected. Do you have any explanation for the different LOS depending performance of both algorithms?
P18, L382 - L384: Concentrations for the lowermost layer rather than conc. at ground?

Do you mean the lowermost layer with concentrations larger than zero? If not, please explain!

P18, Figure 7: Again, MMF doesn't show HCHO values close to zero which means that the main HCHO concentration is found in higher altitudes. MAPA seems to retrieve HCHO closer to the surface. However, P18, L382 - L384 tells us that this conclusion might be wrong. So
I am wondering if you could show a similar figure with surface concentrations only? I have to admit that I am confused by the sentence P18, L382 - L384 and the fact that MAPA finds HCHO concentrations close to zero!

P21, L439 - L440: I am not sure if I understand scheme #3 correctly. In this line, you write about warning flags while you use "erroneous" in Table 4. Please describe this scheme more detailed.

P24, L493 - L494: "Aerosol layers between 2 and 4 km are "invisible"...". This is not correct! An elevated layer will for sure be identified as elevated layer in these altitude regions if aerosols below are negligible. MAX-DOAS might not find the correct altitude but the elevated layer
will be identified for sure showing a small but existing sensitivity.

Figure 12: It is hard to say which profile is the best, especially for the 21. of July. Could you please add a subplot showing the modelled and measured dSCDs at each elevation angle for all scenarios and both algorithms? Maybe this helps to assess better the performance here.

Figure A3: As you have mentioned, the error bars for the scaling factors are larger in winter than in summer.I was wondering if the number of data points in winter is large enough to show a mean daily variation for January (and compare with a similar curve from August)? Do these
curves show a clear diurnal cycle?

References

Tirpitz, Jan-Lukas, Udo Frie, Francois Hendrick, Carlos Alberti, Marc Allaart, Arnoud Apituley, Alkis Bais, u.a. "Intercomparison of MAX-DOAS Vertical Pro le Retrieval Algorithms: Studies on Field Data from the CINDI-2 Campaign". Atmospheric Measurement Techniques 14, Nr. 1 (4. Januar 2021): 1{35. https://doi.org/10/ghx39m.