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review of "Retrieval of tropospheric aerosol, NO2 and HCHO vertical profiles from MAX-DOAS observations over Thessaloniki, Greece" by Dimitris Karagkiozidis et al.

Anonymous Referee #2

Referee comment on "Retrieval of tropospheric aerosol, NO_2, 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-RC2, 2021

The paper "Retrieval of tropospheric aerosol, NO2 and HCHO vertical profiles from MAX-DOAS observations over Thessaloniki, Greece" by Dimitris Karagkiozidis et al., presents results of 2 MAXDOAS profiling retrievals (MMF and MAPA) for 1 year of observation (May 2020 to May 2021) in Thessaloniki. The 2 approaches are presented, with investigations of the impact of different filtering selections, and are compared to available ancillary measurements (AOD from Brewer and CIMEL, aerosols extinction profiles from a few lidar measurements and surface NO2 from in-situ data).
The paper is well written and easy to follow, and its scientific content fits the scope of AMT.
The title is however a bit misleading: we expect to learn about profiles in Thessaloniki, but NO2 and HCHO profiles are never shown in any of the figures! The paper is more about a comparison of the 2 approaches, mostly focusing on VCD and surface concentration, and comparisons to external data, when available (which is not the case for HCHO). The outcome of the study is also a bit confusing, specifying for each case the best regression statistics, but not how to deal with these data if they want to be used. Should an average of both profiling techniques should be recommended? Should we only rely on VCD and surface concentration? Should we use only one of them (eg MMF that provides AVK), but then use the bias to MAPA to estimate a (more) realistic uncertainty? Are the profiles of the 2 algorithm within their estimated uncertainties? (uncertainties of each approach are never mentioned).
It would be good that the authors provide some suggestions in the conclusions.

I would thus recommend some revision of the title and text, with some further geophysical (instead of only statistical) investigation, as described below.
I would also suggest some reordering of Section 3. The results are now presented first for VCD (3.1), then dSCD (3.2), then surface concentration (3.3) and then AVK (3.4). It would make more sense to me to follow the retrieval order: from dSCD, to profiles and AVK, and then VCD and surface extracted from the profiles. Or focusing first on the output products (VCD and surface concentration), and then some diagnostic elements (dSCD and AVK).

specific comments:

The study would allow to present many geophysically results, instead of only showing coherence of 2 (both are possible, see eg. Vlemmix et al., 2015). E.g. answering the following questions:
- how are the profiles themselves (is e.g. the H75 characteristic height (see eg Vlemmix et al., 2015) of NO2 lower or higher than the HCHO and aerosols one? how is it changing over the day and the seasons?)
- how is the variability within the different measured azimuths (is there an heterogeneous situation, as shown e.g. for Athens in Gratsea et al 2016? is it stronger for NO2 than for HCHO, as we would expect?).

Also, to my point of view, the paper is missing the opportunity to make the link with the previously created datasets from this instrument. It would be nice to know how much these profiling results are coherent with approaches used in the past for the VCD estimation (Drosoglou et al., 2017 and 2018, QA4ECV dataset used in Pinardi et al., 2020; Verhoelst et al, 2021; De Smedt et al. 2021). Are results similar or very different in term of VCD? E.g., see comment for P 14, line 338, or for P. 20, line 412.

There is also a lack of reference to literature when presenting the specific results of this study and stating some "realities". (e.g., page 24, line 485 "Since the MAX-DOAS profile retrievals in the UV are sensitive only at altitudes closer to the ground*, where the lidar system is not, the profiles for 360 nm are excluded from the analysis") - *: how can we confirm this sentence?)

It would be good to also show the coherence of the lidar comparisons (Figure 12) with the AOD from Brewer and AERONET. Is the vertically integrated extinction profile coherent with the AOD? (see comment for Figure 12)

Technical comments and corrections:

- Figure 2: please also specify other instruments location.
- Section 2.3 (or 2.6): are the 2 retrievals treating cloud filtering in the same way? are they both starting from a reduced set of cloud filtered dSCD, or is this done within the MMF and MAPA algorithms?
- page 10, line 212: "the progress of the convergence is faster when using an a priori VCD or AOD below the true value" - why is this?
- Section 2.7: specify the location of the ancillary data - how far are they from the

MAXDOAS? and mention the impact of the different fields of views.
- P. 12, line 259: just to have an idea, how many lidar measurements this schedule would represent in the interested time period (May 2020 to May 2021)?
- Section 3: the results are presented separately for the different viewing azimuths (with no clear major difference or explation of difference between MMF and MAPA relative to the azimuth), while in Sect. 4, where the results are "validated", this information is now missing. What is used here? only one of the azimuths or an average of both or a mix of them, depending on the time of the day?
- P. 13, line 305: "the elevation sequences, for which the retrieved AOD from the MAX-DOAS inversion algorithms is greater than 1.5 are filtered-out, since such high aerosol loads are unrealistic for Thessaloniki" - is this a big proportion of data? can this be impacted by clouds, or have these been filtered before?
- P. 13, line 307: "Negative columns can occur in the trace gas retrievals of MAPA within the Monte Carlo ensemble and they are intentionally not removed" - add "at first/by default/..." - is this 8.5% of negative HCHO VCD points already included in the 18% valid MAPA flagged data of Table 3, or to be additionally removed ?
- Table 3: add a third column with the remaining valid data percentage when both algorithms have coincident valid flags (filter #4, used as default in most of this section, if I understood well).
- P. 13, line 317: "an elevation sequence is considered valid as long as it is flagged as valid by both MMF and MAPA. This is the default flagging scheme for NO2, HCHO and AOD at 477 nm" --> this would mean flagging scheme #4 of Table 4, right?
- P. 14, line 324: you mention the Orthogonal Distance Regression (ODR or bivariate least-squares) instead of an Ordinary Linear Regression (OLR or standard least-squares), but in figures 5, 7, 11 you mention linear regression. Please adapt with the correct regression type.
- P 14, line 338 "This is the first time during the Phaethon's operation that the whole elevation sequence is being used in order to derive the tropospheric VCDs more accurately": comment coherence of VCD results obtained here with respect to approaches used in past datasets (see comment above).
- Figure 5: it is difficult to understand from this figure if the larger variability of MAPA results (eg for HCHO and aerosols UV) is related to the different azimuths - is MMF seeing less well the variability among the different azimuths, is MMF too sensitive or is this a false impression? are the SCD showing some systematic (?) larger signal over the city or the sea? or is this just coming from the larger variability in aerosols in the UV ? (if latter explanation is relevant, also add it to P. 16, lines 355- 356).
- P. 19, line 396: consider "Figure 8 shows a typical example of the calculated AVKs for each of the retrieved species. The DoF of this example retrieval
are shown for each species." --> "Figure 8 shows a typical example of the calculated AVKs for each of the retrieved species, including their corresponding DoF."
- P. 19, line 399: "The averaging kernels verify that" - change "verify" to "illustrate" or something similar.
- P. 20, line 412: no other source of independent HCHO is present, but this section could also be a good place to compare results from the 2 profiling algorithms to results of past VCD retrieval methods (see comment above)
- Figure 9: what flagging choice is used to make this figure?
  from this figure, the feeling is that MAPA has systematically lower AOD @477 than the other datasets (a lot of points close to zero), which is not the case for AOD @360. I would say that the comparisons in the UV are better than in the visible...
- P. 21, line 435: "Compared to the CIMEL, MAPA seems to perform slightly better than MMF when its own flagging algorithm is applied to the data, with correlation coefficients of 0.70 and 0.50, respectively." - suggestion to replace by "when each algorithm consider is own flagging, with correlation coefficients of 0.70 and 0.50, respectively (MAPA for case #2 and MMF for case #1)." for more clarity!
- P. 21, line 447: "The AOD derived from the MAX-DOAS, both in the UV and the VIS range, is, generally, underestimated compared to the AOD measured by the CIMEL and

the Brewer" --> add references to other studies showing that! also in P. 22, line 454.
- P. 24, line 476: "Thus, differences in the retrieved extinction profiles are expected, especially at locations with large horizontal inhomogeneities of aerosols" --> is this the case here? having a geophysically analysis (diurnal and seasonal) of the results for the different azimuths would help answer to this question. What azimuth is shown in Figure 12 for MAXDOAS?
- Figure 12: it would be nice to also have a comparison of the integrated aerosols profiles, to compare the lidar AOD to the MAXDOAS ones and to Brewer and AERONET (if available) for those cases.
- P. 26, line 510: what MAXDOAS dataset is shown in Figure 13? all the azimuth angles together?
- Figure 13: how is the fact that the MAXDOAS is situated at an height of 80m is taken into account here?
- P. 26, line 517: Zieger et al 2011 reference is for aerosols comparisons, it should appear in Sect. 4.1 instead of 4.2
- Figure A1: why none of the statistics for NO2 and HCHO correspond to those of Figure 7 black values? I would assume to find the same values in "O4 SF var"?!

References:

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