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## Referee comment on acp-2021-45

Anonymous Referee #1

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Referee comment on "Technical note: Evaluation of profile retrievals of aerosols and trace gases for MAX-DOAS measurements under different aerosol scenarios based on radiative transfer simulations" by Xin Tian et al., Atmos. Chem. Phys. Discuss.,  
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Tian et al. perform investigations on the accuracy of MAX-DOAS retrievals based on synthetic data. The general approaches are very similar to former studies. However, in contrast to the latter, Tian et al. focus on pollution scenarios with exceptionally high AODs and NO<sub>2</sub> VCDs. It therefore provides novel and useful aspects and is worth publishing.

### General comments:

Prior to publication, in particular the presentation of the results and the discussions need to be revised.

The choice and quality of the figures can be significantly improved:

- For many comparisons, the authors created three figures with actual profiles, absolute deviations, and relative deviations, respectively. They decided to only show the relative deviations in the main text and moved the other figures to the supplementary material. I strongly recommend showing the actually retrieved profiles in the main text and (to keep the manuscript concise) move the relative deviation to the supplementary material (e.g. swap Figure 2 and Figure S8, Figure 4 and Figure S12, and so on...). Furthermore, where possible, I recommend to also indicate the PriAM a priori profile in each subplot. Plots of this kind are easiest to read, provide very complete information (relative and absolute deviations can be readily estimated by eye), and allow to directly

- perceive potential impacts of a priori biases.
- Furthermore, the vertical extent of some figures might be enhanced to improve the visibility of profile fine structures particularly close to the surface.
  - Reduce line thickness of the profiles for better visibility where necessary.
  - Regarding labels and legends:
    - the axes tick labels are sometimes wrong (see e.g. horizontal axes in Figure S19)
    - please double check units (see e.g. Fig. 6, where O4 dSCDs are given in molec cm<sup>-2</sup>)
    - Assure readability of legends
    - Avoid long legend labels (an extreme case is Figure 16, as discussed in the specific comments)
  - Where possible, consider applying the same horizontal axes limits in different (sub-)plots.

Some of the wordings in the discussions are not clear to me or at least hard to follow and particularly the final conclusions should be more quantitative. The corresponding paragraphs are listed in the specific comments. A general issue is that authors seem to use the term "systematic deviations" sometimes for the relative differences (hence, considering the sign of the deviations) and sometimes for the general magnitude (independent of the sign) of the systematic deviations. This should somehow be clarified, probably by consistently using the expressions "differences" and "deviation magnitudes" for the first and the second case, respectively.

The authors state, that their findings "explain part of the deviations between the AOD retrieved from MAX-DOAS and sun photometers in previous studies" (P2L5 but also P24L12). First, I do not agree with the word "explain" here, since the presented results simply show the same behavior as observed in former publications. In fact, an actual "explanation" for these systematics has already been proposed by Irie (2008), Frieß (2016), and Bösch (2018): they proposed that biases introduced by the a priori assumptions are responsible for the deviations. Second, Tirpitz et al. (2021) have shown, that, in the case of OEM algorithms, these biases can be accounted for by applying a "partial AOT correction": by taking AVK smoothing effects into account, they estimate the fraction of the AOD that MAX-DOAS inversions are actually able to perceive, and by applying corresponding correction factors, the AOD underestimation observed for MAX-DOAS inversions can largely be removed. Ideally, a "partial AOT correction" should also be performed for the AODs in the presented manuscript (as it is expected to remove large parts of the discrepancies). If the authors think this is out of the scope of their study, they should at least mention the above publications and corresponding explanations/correction approaches.

Keep unit format consistent. Most common: molec<sup>x</sup> cm<sup>-y</sup>

**Specific comments:**

P3L12: "scattered sunlight"

P3L22: remove "aerosol optical depth (AOD) and" here, since the aerosol profiles are the only primary results of the typical inversion.

P4L1: cite Wagner 2004 and Frieß 2006 after "... aerosol extinction."

P5L8-11: Hard to understand. Maybe simplify the sentence at this point: "We compare the aerosol and trace gas profile retrieval results from two MAX-DOAS inversion algorithms (PriAM and MAPA, for details, see below) for different aerosol and trace gas scenarios."

P5L11-12: remove the sentence "For trace gas retrievals..." and improve the explanation in Section 2.1. instead.

Section 2.1: refer to Figure 1 more often in the text to help the reader understand the strategy, e.g.:

P6L1: "A set of atmospheric scenarios (orange box on the very left), ..."

Explain the two strategies here already (please do this carefully also by referring to the Boxes S1 and S2 in Fig.1), such that the reader understands the entire figure before moving on.

P6L5: "SCDs" are not introduced and this should also not be necessary. Change "SCDs" to "DSCDs" here and for all following occurrences of "SCDs". Further, pay attention to consistency: either "dSCD" or "DSCD" (e.g. P6L19)

P6L14: "assumed input profiles" for consistency.

P7L11: "Section 3.1.2"

P7L16: "wavelengths of 360 nm"

P7L18: The described profile shapes were generally used for different investigations, not only as a priori, right? Maybe keep this more general and remove "as a-priori".

P8L11: "a priori" instead of "a-priori". Check further occurrences throughout the manuscript.

P8L16: "were PriAM and MAPA, as listed ..."

P10L17: AODs = 3 are included or? So it should be AODs less-equal 3 instead of less than 3.

P11L1: Sentence seems messed up: multiple references to Table 1 and a bracket out of place. Please correct/rephrase.

P11L3-8: I do not understand the criteria on which the authors took the decisions here. This needs to be explained in more detail. Currently, I do not see much value in the presented side investigation. Therefore, alternatively, the corresponding investigation might be removed completely, and instead only the four profiles of relevance for the rest of the study might be introduced in the text and in Table 1. This might also avoid some confusion.

P11L19: "In this Section the effect..."

P13L8-11: I cannot follow. On the one hand, the relative deviations (I guess it should be the "relative deviation magnitude") increases with AOD but then it does not? Please clarify.

P14L17: Also add the scale height. It might be useful to add a "default a priori profile"-row

to Table 1 with the relevant properties.

P15L1-3: It might be interesting to briefly discuss the motivation for this approach and particularly its relevance for real measurements, where there is basically no information on the vertical distribution or the AOD prior to the inversion. Do have any strategy in mind on how real retrievals might be improved e.g. by iteratively adapting the a priori profile (which is btw. quiet arguable as it violates the OEM principle)? It might be worth discussing this at least at some point (Conclusions?)

P15L8-9: "no effect" doesn't seem right here. According to Figure 4, for the Boltzmann and the Gaussian input profiles it has "little effect", while for the exponential input profiles there are significant differences right? Please clarify.

Section 3.1.3: What are the values of the off-diagonal elements of Sa? Btw. the default a priori covariance information also be included in Table 1.

P16L1: what does "correlation" mean here? Correlation coefficient?

P16L5-6: Shouldn't this be the other way round? Also, it is not ideal to talk of "limits" in the context of OEM approaches. I propose: "This is due to the fact that biases towards the a priori profiles are reduced with increasing Sa values."

P16L7: Give an approximate altitude for "upper layers".

P16L8-11: In my opinion, this is the major finding of the section. However, it only considers the correlation coefficient. What about the actual agreement (e.g. in terms of RMSD). This is probably the most important quantity to minimise.

P16L17: AOD less-equal than 3 (?)

P17L8: Remove double full stop.

P17L13: comma after "AOD"

P17L14-19: I would expect the different ways of how a priori information is incorporated in the two retrievals as a major reason: for PriAM this is of course the a priori profile and the a priori covariance. For MAPA a priori assumptions are incorporated in the form of prescribed profiles described few parameters. This might be added as another potential reason.

P18L5: Would be helpful to give the applied values for SAA and AP in brackets here again.

P18L7: "...using the "correct" SSA and AP values (hence, the same values as they were applied in the corresponding O<sub>4</sub> DSCD simulations)"

P19L1: What do the numbers "0.01 to 1.5" represent? I guess these are absolute deviation magnitudes in the extinction coefficient? Please clarify and add units if necessary.

P19L5: Add the 5 VCD values in brackets here again.

P19L6: Add one sentence here again on "S1" and "S2" to remind the reader of approximate meaning.

P19L21: Shouldn't this be "Fig 10" instead of "Fig. S10"?

P19L19: "..., the magnitude of absolute deviations between the retrieved ..."

P19L20: "... with increasing NO<sub>2</sub> VCDs. However, the relative deviations..."

P19L19 – P20L1: I would say, the relative deviations generally increase with AOD, don't they?

P20L1: What is meant by "The systematic deviations here"? The largest deviation magnitudes? Absolute or relative? Please clarify.

P20L8-13: Do these findings apply for both algorithms or only for PriAM? Please clarify.

P20L13 Remove either "uncertainty" or "covariance"

P20L21: Start a new paragraph before "The NO2 profiles..."

P21L4-6: What is meant by "singular values". Outliers in single layers? I do not see such things in the figures. Please clarify.

P21L17: "...value of the Sa diagonal..."

P23L5-8: Similarly as for the AOD (see general comments) I would suspect a priori biases as the reason for the systematic deviations. It might be out of the scope of the study, but I encourage the authors to try a corresponding correction: Convolute the input profiles with the retrieval AVKs, recalculate the VCD from the smoothed profile, and compare this "a priori bias-corrected" true VCD to the retrieved VCDs. Do the systematic deviations disappear?

P23L20: add VCD range here

P24L5: Please provide at least some order of magnitude or a range of deviations.

P24L12-14: See general comment regarding systematic deviations between MAX-DOAS and sunphotometer observations. Please discuss the actual reasons here and give credits to the corresponding former publications.

P24L17: "...in the RTM model. It..."

P25L4-6: This is very likely due to the corresponding reduction of a priori biases. Might be added as a potential explanation.

P26L7: What does "single outliers" mean. Single profiles? Single layers? Please explain further.

Figure1: Change upper green diamond to "Comparison of "input" and retrieved aerosol profiles". Change lower green diamond to "Comparison of "input" and retrieved trace gas

profiles”

Figure 2 caption: “where the retrieved AOD exceeds 2”. Shouldn’t this be “3”?

Figure 5: Legend: add a square root over “Sa” or a square to the numbers (0.06<sup>2</sup>, 0.1<sup>2</sup>, ...).

Figure 6: Units should be molec<sup>2</sup> cm<sup>-5</sup>

Figure 7, legend: remove typo “deviatiobs”

Figure 10, end of caption: “...shown at the top.”

Figure 13: Might be useful to add the default a priori uncertainty as error bars or shaded area.

Figure 16: Legend is extremely bulky making it harder for the reader to understand the figure. One column might be enough since absolute and relative deviations are shown in separate subplots. Furthermore, the legend might be equipped with a title like “Deviations between retrieved and input NO<sub>2</sub> VCDs”. Labels can then be reduced to something like “Priam\_S1, AOD 0.3”.