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Atmospheric Measurement Techniques
Discussions

Interactive comment on "Intercomparison of MAX-DOAS Vertical Profile Retrieval Algorithms: Studies using Synthetic Data" *by* Udo Frieß et al.

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We thank Referee #3 for his detailed comments. We reply to the individual comments point by point, with the original comments shown in *italic*, our replies in roman, and changes to the manuscript in **bold**.

However, at certain times I found points needing clarification. For example, I wonder how the NASA algorithm using only RTM calculations with Rayleigh scattering, works to yield aerosol profiles; O4 optical depth could be assigned for each layer, but I believe only RTM calculations with aerosols can connect the O4 information and aerosols.

The description of the NASA algorithm has been updated with a more detailed explanation of the approaches for aerosol and trace gase profile retrieval. The revised

NASA algorithm description has been uploaded to the public discussion page as a supplemental document.

Secondly degrees of agreement with surface values (section 6.6) should be compared to those with vertical total columns. The last sentence of Abstract and the second sentence of Conclusions focused on difference quantification of "concentrations", but implication for column values would be similarly or even more important, considering MAX-DOAS is heavily used for satellite validation.

In order to bring the accuracy of surface value and total column into relation, we have added the following statement to Section 6.6: **For the prescribed profile scenarios, retrieved aerosol surface extinction (mean regression coefficient from all algorithms $\bar{R} = 0.903$ at 360 nm and $\bar{R} = 0.825$ at 477 nm) shows a better agreement with the true value that the AOT ($\bar{R} = 0.874$ at 360 nm and $\bar{R} = 0.803$ at 477 nm). The opposite is true for trace gases, where the agreement of the total column ($\bar{R} = 0.969$ and $\bar{R} = 0.955$ for HCHO and NO_2, respectively) is better than for the surface mixing ratio ($\bar{R} = 0.894$ and $\bar{R} = 0.780$).**

1. Page 1, line 12. The authors state that the values are root mean squares, but they are not described much in detail in text (section 6.6).

We have added a paragraph discussing the RMS of surface and total column values to Section 6.6, see above.

2. Page 2, line 34. A posteriori modelled "d"SCDs? Same for the rightmost green box in Figure 1?

SCDs has been replaced with **dSCDs**, both in the text and in Figure 1.

3. Page 3, equation (4): What is S_e? How were they assumed in the OEM calculations? The dSCD errors listed in Table 6 correspond to this?

We have added the following statement after Figure 4: **Here S_ϵ is the measurement covariance matrix, which, under the assumption that the measurements are in-**

dependent, is a matrix with the squares of the measurement errors (specified in Section 6.1 and Table 6) as diagonal elements and zero values elsewhere.

4. Page 10-11. Description of NASA algorithm should be elaborated as mentioned earlier. In Page 11, line 2, Are there cases where less than four measurements are available, for this synthetic-data-based study? Page 11, line 6. O4 dSCDs at low angles are used instead of the aerosol retrieval results ? how this approach works without RTMs is difficult to understand.

The NASA algorithm description has been updated, see our reply to the general comment above.

5. AER8, 9, and 10 in Table 3 and 5. Parameters for fog/clouds (particularly for single scattering albedo) are same as those for aerosols?

Yes, the optical parameters are the same. We are aware that in reality optical properties of cloud droplets are significantly different from those of aerosols, and there is of course also a high variability for different kinds of aerosols. However, it is assumed here that aerosol properties are perfectly known and are the same for forward modelling and inversion. So the choice of the optical properties should have very little influence on the results.

6. Bottom panels of Figure 3 for gases: Results for all scenarios with different aerosol profiles are included?

Yes, the following sentence has been added to the caption of Figure 3: **For HCHO and NO_2, results for all scenarios with different aerosol profiles are included.**

7. Page 20, lines 1-3. The authors should mention that O4 profile shape is heavily weighted to low layers.

We have added the following sentence to the discussion of the vertical sensitivity in the first paragraph of Section 6.2: **This is a result of the measurement geometry and, in case of aerosols, also of the fact that the O_4 vertical distribution is heavily**

weighted to the surface.

8. Page 20, line 13. Better specifically mention as "synthetic" measurement vector (y)? Same for x axis label of Figure 9. Y-axis label in Figure 9 should be better mentioned as a posteriori modeled dSCDs?

The sentence on page 20, line 13, stating that the agreement between the measurement vector $\mathbf{y}$ and the measurement vector $\mathbf{F}(\hat{\mathbf{x}})$ is an important indicator for the level of convergence, is valid not only for synthetic studies but in general for all applications. We would therefore rather not add the term "synthetic". It is stated in the caption of Figure 9 that the y-axis shows a posteriori dSCDs, and adding this to the y-axis label would make the label too lengthy. To make clear that we refer to simulated measurements from the synthetic dataset whenever we state "measurements", we have added the following statement to Section 6.1: **In the following, we refer to this synthetic dataset as the measured dSCDs.**

9. Page 20, line 3. Any reasons for the underestimation of O4 at 477 nm?

We assume that you refer to page 21, line 3. One of the reasons might be that the constraint of the retrievals by the a priori covariance might be too strong specifically for the PriAM algorithm. However, the investigation of the reasons for deficiencies of the individual algorithms is beyond the scope of this study, and we have no knowledge about the reasons for the underestimation of O_4 at 477 nm by the PRIAM algorithm.

10. Figure 10 and 15. Y-Axis range for Slope is better zoomed to narrower range?

Our intention was to have the same y-axis ranges for slope and regression coefficients in Figures 4, 10, 15, 18, and 21. This has now been changed and the axis ranges now better match the range of the data points.

11. Figure 13 caption. Legend for coloured symbols corresponding to aerosol scenario is not found.

The legend now has moved to the top of the Figure, with a larger font size for better readability.

12. Figure 14. My guess is that MAX-DOAS gas determination would be difficult in the AER2+TG7 scenario. Can the scenario be identified in the plot for some discussion?

The AER2/TG7 scenarios (shown as green circles) do not pose any particular difficulty for any of the algorithms. In contrast, some of the OEM algorithms (BEPRO and BOREAS) have difficulties with uplifted profiles during fog (AER8/TG7; green diamonds).

13. Page 28, lines 1-5. How the failure in retrievals in aerosol/cloud affected the gas retrievals? If correct aerosols profiles are given, better agreement is obtained?

In general, the trace gas retrieval is surprisingly stable even if the aerosol profiles appear to be unrealistic, a finding that has also been confirmed by real measurements. We focused on the performance of the algorithms based on the processing chain that is also applied to field measurements (i.e., using the aerosol profiles from the retrieval based on O_4 dSCDs as a constraint for the trace gas retrieval), and tests using the 'true' aerosol profile as a constraint for the trace gas retrieval are beyond the scope of this study.

14. AER0 and TG0 cases for bePRO, HEIPRO, MMF, and PROAMF in Figures 16 and 17. As mentioned in page 30 lines 7-8, a positive bias is present. This might be fatal for satellite validation in clean region. Can they be easily screened out during post error analysis, for example, comparison with largest dSCD values?

The bias for low (or zero) aerosol and trace gas scenarios from the OEM algorithms is indeed quite large for the settings chosen in this study. For atmospheric measurements, this can be overcome by either using smaller a priori concentrations/extinctions during clean air conditions and/or by increasing the a priori covariance. It is, however, crucial to investigate potential biases and other error sources, and to minimise these by choosing optimal settings for each individual field site and for each algorithm.

15. Y-axis of Figure 16. AOT is used throughout text?

AOD has been replaced by AOT in Figure 16.

16. Page 33. Degrees of agreement with surface values (section 6.6) should be compared to those with vertical total columns.

See our reply to the general comment above.

17. Section 6.7. Any time loss during data I/O for some algorithms?

Yes, the time for data I/O has been included in the benchmark. This should, however, only be significant for the NASA algorithm with a processing time in the order of milliseconds.

18. Page 36, line 7. bePRO

This has been corrected.

19. Page 36, line 10. have shown

This has been corrected.

20. Page 37, line1. Do the authors mean "direct-sun" observation here?

We are not referring to direct sun observations here, but to observations close to the sun (e.g., in the aureole region), which can cause difficulties due to stray light within the telescope, or unintentional intersection of the field of view with the solar disc. Also, the aureole region is particular sensitive to the aerosol phase function and a wrong choice of the aerosol optical parameters for the retrieval might introduce larger errors than for measurements elsewhere in the sky.

21. Recommendation learnt from this study should be listed in Conclusions?

The following statement has been added to the conclusions: **As a result of this study, the MMF and the MAPA algorithms, both showing best performance in terms of reconstruction of the atmospheric state and computational speed,**

were selected as profile algorithms for the FRM_4DOAS centralised near-real-time algorithm for a harmonised processing of MAX-DOAS data, which is planned to be made available to the community in the near future.

Please also note the supplement to this comment:
https://www.atmos-meas-tech-discuss.net/amt-2018-423/amt-2018-423-AC4-supplement.pdf

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