Author reply to Referee #2

Tim Bösch et al.

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We thank Referee #1 for carefully reading our manuscript and for the helpful comments which will improve the quality of our manuscript. We will reply to the comments point by point.

Legend:

- referee comments
- author comments
- old text from the manuscript
- changed text in the manuscript

This paper reports a new MAX-DOAS profiling algorithm detailedly. The algorithm is based on a scientific reasonable method. The results have good correlation with the results from the other instruments.

Thank you very much for the positive comment.

However, from the paper, it appears that the algorithm is similar to the other profiling algorithms based on the optimal estimation method. The title of this paper is about a NEW algorithm, so you should highlight what is really NEW and innovative in your algorithm, and what are the advantages comparing to the other MAX-DOAS profiling algorithms. These points should also be included in the Abstracts.

To the authors knowledge, the approach of the aerosol retrieval is completely new. The trace gas retrieval, presented in this manuscript, is based on the optimal estimation (OE) method and is similar to retrievals used in other studies. However, the applied approach on improving the regularization ratio empirically as well as the a priori pre-scaling option are new and might help the community to reduce oscillations and wrongly weighted a priori constraints.

We will follow the suggestion of the reviewer by adding the following lines to the abstract:

The aerosol profile retrieval is based on a novel approach in which the absorption depth of O_4 is directly used in order to retrieve extinction coefficient profiles instead of the commonly used perturbation theory method. The retrieval of trace gases is done with the frequently used optimal estimation method but significant improvements on how to deal with wrongly weighted a priori constraints and for scenarios in which the a priori profile is inaccurate are presented.

Furthermore, the latter point will be also mentioned in the Introduction:

In order to improve the standard OE method for trace gases, a simple way of changing the weighting between a priori and measurement constraints is introduced by varying a regularization factor so that oscillations are minimized. Additionally, the usage of a priori pre-scaling will be highlighted as one way of improving results when the a priori profile is far away from the real atmosphere. In Figure 4, readers cannot easily distinguish between the curves corresponding to E2 and E3. Different line styles should be used for the curves of different episodes (also in the other similar figures). In the right-hand chart, the pre-scaled a priori profiles ought to be depicted.

As suggested, the linestyles were changed and the pre-scaled a priori profiles were included. The following four figures were adapted for this purpose and will be added to the new manuscript.



Figure 1: (Changed version of manuscript Figure 4) Retrieval results with a fixed (left) and a pre-scaled a priori profile (right) with varying Tikhonov parameters γ for SNR = 3000. Small γ values mean less smoothing of the resulting profiles.



Figure 2: (Changed version of manuscript Figure 7) Retrieval results with a fix (left) and a prescaled a priori profile (right) with g factors. Small g values mean less measurement weighting for the resulting profiles.



Figure 3: (Changed version of manuscript Figure A2) Retrieval results with a fix (left) and a pre-scaled a priori profile (right) with varying Tikhonov parameters γ for SNR = 3000. Small γ values mean less smoothing of the resulting profiles.



Figure 4: (Changed version of manuscript Figure A9) Retrieval results with a fix (left) and a pre-scaled a priori profile (right) with g factors. Small g values mean less measurement weighting for the resulting profiles.

Moreover, I cannot understand about how are the a priori profiles pre-scaled.

For both, the aerosol and the trace gas retrieval, the corresponding a priori profiles are scaled so that the AOT and VCD of the new a priori profiles match the values found from an initial calculation with a "zero"-profile and from the 30° dSCD measurement for aerosols and trace gases, respectively. In order to clarify this approach, the aerosol pre-scaling description will be extended by the following lines in Section 4.1.1:

In Equation 15, the a priori profile x_0 is set to 0 but the remaining terms stay unchanged in order to retrieve a reliable AOT value without limiting the solution by a certain profile shape.

The AOT from this pre-calculation is used to scale the a priori profile for the true run.

The AOT from this pre-calculation is used to scale the a priori profile for the main run by calculating a scaling factor from the initial a priori AOT and the new value which is applied to all initial extinction coefficients before the main inversion.

In Section 4.1.2, the following lines will be changed in the trace gas pre-scaling description:

This vertical column density V is used as a pre-scaling values for the a priori profile.

The new a priori profile is scaled to match this vertical column density V by calculating a scaling factor from the initial and the retrieved V which is applied to all initial concentration values before the main inversion.

In the chapter about CINDI-2 campaign (4.3), the results are compared with the results from other instruments. However, it is also important to compare with the MAX-DOAS result from the same instrument but retrieved with the other algorithms.

We fully agree with the reviewers suggestion. However, the BOREAS algorithm participated in a comparison study for synthetic data and real data which will pe published by Frieß et al. (2018) and Tirpitz et al. (2018), respectively. In both studies, several community algorithms are presented and compared to each other so that we decided to focus only on a validation study with ancillary measurements instead of repeating comparisons shown in the other two papers.

Some well-known and fundamental introductions can be simplified. For example, it is unnecessary to explain the definition of single scattering albedo in detail and show the equation.

We follow the reviewers suggestion by removing the definition of single scattering albedo and slant column density from the manuscript.

In the description of the algorithm, it is better to use the symbols that are commonly used in the related papers. For example, in Equation (3), it is better to use "AMF" instead of "M", "SCD" instead of "S", and "VCD" instead of "V". In Equation (5), you can just use "BAMF" instead of the curlicue M.

The authors believe that one letter variable symbols make the understanding of longer equations easier. Furthermore, these variables are also used in the literature (cf. Platt, 1994) and in other publications (cf. e.g. Marquard et al., 2000). One exception is M for the air mass factor which was chosen because A is additionally used for the averaging kernels.

Minor corrections:

Page 1, Line 4: "in a second part" \rightarrow "in the second part".

Will be changed as suggested.

Page 9, Line 5: If Δy is a vector, then it should be described as "has N·M elements" instead of "has the dimension N·M×1"; otherwise it should be described as a matrix.

Will be changed as suggested.

Similarly, Line 10, the state vector Δx should have "L elements". Line 11, "N·M×L" \rightarrow "(N·M)×L".

Will be changed as suggested.

Page 20, Line 14: "CINDI2" \rightarrow "CINDI-2".

Will be changed as suggested.

References

- Marquard, L. C., T. Wagner, and U. Platt (Jan. 20, 2000). "Improved Air Mass Factor Concepts for Scattered Radiation Differential Optical Absorption Spectroscopy of Atmospheric Species". In: Journal of Geophysical Research: Atmospheres 105.D1, pp. 1315–1327. ISSN: 2156-2202. DOI: 10.1029/ 1999JD900340.
- Platt, Ulrich (1994). "Differential Optical Absorption Spectroscopy (DOAS)". In: Air Monitoring by Spectroscopic Techniques. 127. New York: John Wiley & Sons, pp. 27–84. ISBN: 0-471-55875-3.