Final response to referee comments on paper amt-2019-243

First of all, we would like to thank reviewer #2 for his/her constructive comments, which helped to improve the manuscript. Below we give answers and clarifications to all comments made by the referee (repeated in italics).

Anonymous Referee #2

General comments

Reviewer: *The authors present a scientific algorithm to simultaneously retrieve carbon monoxide and methane from TROPOMI onboard Sentinel-5 Precursor. I understand that this activity is important to calibration and validate both of TROPOMI spectra and operational products. However, it is unclear that what is the object for developing the proposed algorithm or how is the difference between the proposed algorithm and the operational one. In this paper, a lot of demonstrated results are described. Unfortunately, it is hard to understand the usefulness of this algorithm. It is easy to understand, if this paper focus on the validation of TROPOMI operational products. Several topics are described in this paper but the relevance between these topics are poor. Of course, the individual topics are important. So, I recommend the authors will reconstruct the frame of this paper.*

Authors: We have added details of the objectives of this new algorithm to the abstract and the introduction. The differences to the operational algorithm are described in Section 4.1. The goal of the paper is to introduce the TROPOMI/WFMD algorithm including error assessments based on synthetic data and validation with independent reference data to show that the algorithm is suitable to retrieve XCO and XCH_4 from real TROPOMI data well within the mission requirements after quality filtering. The good global agreement of our scientific products with the operational products for the analysed example cases further underlines the quality of the presented algorithm. The possibility to learn from the differences in detail is one of the advantages of having several distinct retrieval algorithms for each analysed atmospheric constituent at hand. Perhaps the most striking new feature of TROPOMI is the capability to readily detect emission sources in a single satellite overpass due to its unique combination of high precision, spatiotemporal resolution, and coverage. This enables new application areas and has the potential to advance emission monitoring and air quality assessments to an entirely new level because of the daily recurrence.

The leitmotif of Section 4 is to present initial results concerning comparison to the operational products and detection of emission sources. However, it is not the intention of the manuscript to give final answers in these areas, but rather to describe the objectives and outline the future potential as described in the conclusions. The comparison to the operational products is limited to example cases to demonstrate the broad consistency of the algorithms and the emission source analysis focusses on qualitative examples to demonstrate the new capabilities. A complete verification of the operational algorithms and the detailed quantitative reinforcement of the analysis of specific emission sources is out of the scope of this manuscript and will be discussed elsewhere. Along these lines, we have changed the name of Section 4 to "Initial results using real TROPOMI data". We have also modified the abstract and the introduction to make this more clear. Please, see also the answers to the specific comments for more details.

Specific comments

Abstract

Reviewer: *Describe the character of proposed science algorithm. Especially, the comparison between the proposed algorithm and the operational one.*
Describe the motivation or object for developing proposed algorithm.

Authors: The objectives have been added to the abstract in the revised version including the intention of mutual verification of the operational and the presented scientific algorithms.

Reviewer: *Describe a full word of "DOAS".*

Authors: Has been added.

Reviewer: *Page 2, line10: What is a "reference data".*

Authors: Has been changed to "validation data" for the sake of clarity.

Reviewer: *Page 2, line13: Why emission sources have to be identified? Describe the object or background.*

Authors: We have added a sentence that the detection of emission sources in a single satellite overpass has the potential to advance emission monitoring and air quality assessments to an entirely new level.

Reviewer: *I understand that one of target for developing this scientific algorithm is to validate the operational TROPOMI XCH4 and XCO products. If so, it might be described in.*

Authors: We have added a sentence that *mutual verification* of the operational and the presented scientific algorithms is one of the objectives. We think that the term *verification* is more suitable than *validation* when comparing satellite data sets because satellite data should not be considered as ground truth which is needed for validation.

Introduction

Reviewer: *Page 4, line 9 to line 15: It is unclear what is the requirement of a scientific algorithm? I understand that validation of operational products, calibration of TROPOMI spectra, and reduce the random and systematic error of XCH4 and XCO with scientific algorithm are first objects. Second is new findings with scientific algorithm. If so, describe more clearly.*

Authors: Details of the objectives of this new algorithm are now described more clearly in the last paragraph of the introduction, which now reads: "Here we introduce a scientific algorithm to retrieve CO and CH_4 simultaneously from TROPOMI that has the objective to complement the operational algorithms in the sense described above and to provide new geophysical insights, whilst performing within the mission requirements concerning random and systematic errors at the same time. The presented scientific algorithm differs from the operational algorithms in several respects (Landgraf et al., 2016; Hu et al., 2016) (see also Section 4.1 for a summary of the differences) and the corresponding products are thus predestined to be used together with the operational products in an ensemble approach. After a thorough description of the algorithm including error characteristics based on synthetic data and validation with independent reference data, we present first results of our new algorithm for both trace gases demonstrating the broad consistency with the operational products for example cases and the potential to advance the new application fields, for which TROPOMI's groundbreaking features pave the way."

WFM-DOAS retrieval algorithm

Reviewer: *Figure 1, It is unclear the coverage of gray hatch. Add table for these coverages.*

Authors: We have added the extent of the fitting windows to the caption of Figure 1 in the revised version.

Reviewer: *Table 2, Describe the meaning of "T", "p", "BL", "R", "τ".*

Authors: We have changed T to temperature, p to pressure, and BL to *boundary layer* in Table 2 for a better understanding. The cloud optical thickness τ and the effective radius R are now explained in the caption.

Reviewer: *Figure 5, Describe the full word of "cum", "cir"*

Authors: The abbreviations for water clouds (cumulus) and ice clouds (cirrus) are explained in the figure caption in the revised version.

Reviewer: *Figure 6, Describe the meaning of numbers for surface type.*

Authors: The meaning of the labels has been added to the figure caption in the revised version: 1 Crops, Mixed Farming; 2 Short Grass; 3 Evergreen Needleleaf Trees; 4 Deciduous Needleleaf Trees; 5 Deciduous Broadleaf Trees; 6 Evergreen Broadleaf Trees; 7 Tall Grass; 8 Desert; 9 Tundra; 10 Irrigated Crops; 11 Semidesert; 12 Ice Caps and Glaciers; 13 Bogs and Marshes; 14 Inland Water; 15 Ocean; 16 Evergreen Shrubs; 17 Deciduous Shrubs; 18 Mixed Forest; 19 Forest/Field Mosaic; 20 Water and Land Mixtures.

Reviewer: *Page 12, line 8 to 15: In the other algorithm to retrieving the XCH4 and XCO used O2A spectra, to identify the photon path with precisely. However, this algorithm is not employed the O2A spectra to identify the photon path. Instead of O2A spectra, this algorithm used the ECMWF-Based mole fraction computation. The authors are concluded that the proposed algorithm is more faster and accurate than that of O2A based processing system. However, it is not quantitative. The authors have to assess more quantitatively.*

Authors: The respective text passage has been changed accordingly and now reads "... For these reasons, O_2 is a barely sufficient proxy for the lightpath in the $2.3\,\mu$m spectral range in a scattering atmosphere. For example, the O_2 errors for the scattering scenarios *aerosols/extreme in boundary layer* and *clouds/cirrus* from Table 2 are −5.40% and −7.54%, respectively. Hence, the O_2 underestimations are considerably larger than the corresponding errors for CH_4 and CO, which would lead to distinct overestimations of mole fractions obtained from the O_2-proxy approach in the presence of strong scatterers.

In addition to the better accuracy of the ECMWF-based mole fraction computation, this approach is also faster, because the oxygen fit and the interband coregistration mapping can be omitted. As a consequence, the fitting procedure is about twice as fast without the normalisation by O_2. The ..."

Reviewer: *Page 13, line 22: Make table for "all 25 features".*

Authors: The 25 features are listed in the following sentence. This has been made more clear in the revised version.

Reviewer: *Page 15, Figure 8: What is the meaning of "QUAL=1"?*

Authors: QUAL=1 are excluded scenes of the implemented machine learning quality filter described in this section. We have added the explanation to the figure caption.

Results

Reviewer: *Page 24, line 4: Correct the capital position.*

Authors: Has been changed to "Shortwave Infrared CO Retrieval (SICOR)" in the revised version.

Reviewer: *Page 24, line 6: typo "amd".*

Authors: Has been changed.

Reviewer: *Page 25, Figure 15: Why the yield rate for XCH4 is drastically different between WFMD CO and Operational CO?*

Authors: As described in the main text describing Figure 15, the operational CO algorithm exhibits a better coverage as it can handle a larger amount of cloudiness.

Reviewer: *Page 27, Figure 18: How is the operational products? Is it possible to identify the emission sources with operational products?*

Authors: We have added a Figure showing the operational product and a related discussion in the revised version: "For comparison, Figure 18 also shows the operational product in addition to the TROPOMI/WFMD results. As the operational product is available as total CO columns, the corresponding mole fractions XCO were generated in the same way as for the scientific product by division of the total CO columns by the dry air columns obtained from ECMWF. The comparison demonstrates that the enhancements due to the analysed emission sources can be typically identified in both data sets. However, as a consequence of the different spatiotemporal sampling, the enhancement over some point sources is somewhat more pronounced in the WFMD product. A possible reason for this is the additional utilisation of cloudy observations in the operational SICOR product, which may be associated with reduced surface sensitivity under certain conditions reflected in the averaging kernels of the corresponding measurements."

Reviewer: *Figure 19 to figure 22 are almost same information. These figures are just illustration. Make more clear sentence.*

Authors: These figures show examples of detection of emission sources in a single overpass for different regions, source types, source strengths, and trace gases. It is important to demonstrate that sufficiently large emission sources can be detected reliably. These various examples underpin that detection is the rule and not the exception. This enables new application areas like emission monitoring and air quality assessments as described in the introduction. A similar statement has also been added to the abstract in the revised version. See also the answer to the general comments.

Conclusions

Reviewer: *Page 33, line 10, The sentence "for example with respect to striping" is not touched on this paper. Adding the reference or explanation*

Authors: Striping in flight direction for single overpasses is introduced in Section 4.2.1 when discussing Figures 19 and 20. The meaning is made more clear in the conclusions of the revised version.