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

First of all, we would like to thank reviewer #1 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 #1

Specific comments

Reviewer: *p.4. line 15 : Details of the goal and the contribution of this new algorithm are missing in the introduction. Also, as you mentioned in your abstract EGU 2019, you should said something similar about "We present first results for both CO and CH4 trace gases obtained using the new version v1.2 of the scientific retrieval algorithm WFM-DOAS".*

Authors: We have modified the introduction accordingly. The last paragraph of the introduction 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."

Reviewer: *p.6, line 9 : "the look-up table is only covering direct nadir conditions". Why ?*

Authors: The explanation is added to the manuscript, namely to limit the dimension of the look-up table to a reasonable size. With n sampling points for the viewing zenith angle, the look-up table size would increase by a factor of n.

Reviewer: *p.8, line 10 : The scenario class of profiles are extracted from the radiative transfer model MODTRAN. Why from this RTM ?*

Authors: We have modified this text passage to better represent the origin of the profiles. Anderson et al. (1986) have designed this data base to be incorporated in radiative transfer models in general. It was chosen because the included profiles are considered realistic as they are based on measurements and theoretical predictions. The passage now reads: "In order to examine the sensitivity to vertical profile variations, the scenario class of *Profiles* includes several realistic model atmospheres based on measurements and theoretical predictions (Anderson et al., 1986), with all methane profiles scaled to have surface values of 1850 ppb in each case to better represent current atmospheric conditions."

Reviewer: *p.8, line 11 : "which differ from the US Standard Atmosphere" but how much ?*

Authors: A visualisation of the different vertical profiles can be found in Appendix A of Anderson et al. (1986). This information is added to the manuscript.

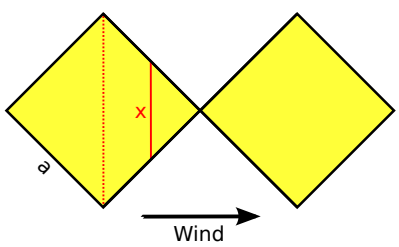
Reviewer: *p.13, line 20 : "20% of the training data are randomly drawn and retained as test data". How did you choose 20% ?*

Authors: A split with 20% test data is widely used. This is explained in the revised version with two example references (Suthaharan, 2016; Hino et al., 2018).

Reviewer: *p.31, line 5 : how did you measure the plume width perpendicular to the wind direction ?*

Authors: The estimation of the plume width is described in more detail in the revised version. The corresponding text passage now reads: "The plume width is on the same order of magnitude as the instrument's spatial resolution and the enhancement is thus calculated for the plume scene passing the quality filter which is nearest to the fire origin. As the wind direction is approximately perpendicular to one of the scene diagonals, the corresponding plume width $x_\perp$ is estimated by $\frac{a}{\sqrt{2}}$ assuming a quadratic scene with a side length a of about 7 km."

Sketch:



Technical comments

Reviewer: *p.2, line 19 : "Moreover, it" → "Moreover, CO" as you are talking about O3 just before...*

Authors: Has been changed in the revised version.

Reviewer: *p.3, line 22 : I would add a reference on this sentence about the high precision of TROPOMI.*

Authors: The reference for the whole paragraph including the high precision statement is the cited paper Veefkind et al. (2012).

Reviewer: *p.4, line 18 : is a linear-least squares method*

Authors: Has been changed in the revised version.

Reviewer: *p.4, line 19 : vertical profiles of trace gases.*

Authors: This sentence shall also comprise temperature and pressure profiles. Therefore, the original phrasing was retained unchanged.

Reviewer: *p.5, line 27 : where T is the matrix transpose.*

Authors: Has been added in the revised version.

Reviewer: *p.8, line 14 : acronym of ASTER and USGS should be mentioned here and not after.*

Authors: The acronyms are explained at this place in the revised version.

Reviewer: *p.11, line 11 : have also to be implemented → have to be implemented*

Authors: Has been changed in the revised version.

Reviewer: *p.11, figure 6 : what is the meaning of the label for the surface type (range from 1 to 20). I did not find the information in the references mentioned in the paragraph 2.4.*

Authors: The labels are explained in Appendix 6 of the Global Land Cover Characterization (GLCC) readme file. The meaning of the labels has been added to the figure caption in the revised version.

Reviewer: *p.13, line 12 : acronym of VIIRS is defined pages 15 and 30 but must be mentioned here too*

Authors: Has been done in the revised version.

Reviewer: *p.27, line 11 : do you have a reference for this percentage ?*

Authors: We have added two references in the revised version. The sentence now reads: "The resulting converter gas predominantly consists of CO ($\approx 70\%$) (Ishioka et al., 1992; CarbonNext, 2017).

Reviewer: *p.33, figure 23 : we do not see very well the cyan color on this figure. Same case for "Edwards" in red letters.*

Authors: The colours have been changed in the revised version for the sake of better visibility.

References

Anderson, G. P., Clough, S. A., Kneizys, F. X., Chetwynd, J. H., and Shettle, E. P.: AFGL Atmospheric Constituent Profiles (0-120 km), Environmental Research Papers, NO. 954, AFGL-TR-86-0110, `https://apps.dtic.mil/dtic/tr/fulltext/u2/a175173.pdf`, 1986.

CarbonNext: Map of relevant CO2 and CO containing gases, `http://carbonnext.eu/Deliverables/_/D1.1MapofrelevantCO2andCOcontaininggases.pdf`, 2017.

Hino, M., Benami, E., and Brooks, N.: Machine learning for environmental monitoring, Nature Sustainability, 1, 583–588, `https://doi.org/10.1038/s41893-018-0142-9`, 2018.

Ishioka, M., Okada, T., and Matsubara, K.: Formation and characteristics of vapor grown carbon fibers prepared in Linz-Donawitz converter gas, Carbon, 30, 975–979, https://doi.org/10.1016/0008-6223(92)90124-F, 1992.

Suthaharan, S.: Machine Learning Models and Algorithms for Big Data Classification, Springer, New York, 2016.

Veefkind, J. P., Aben, I., McMullan, K., Förster, H., de Vries, J., Otter, G., Claas, J., Eskes, H. J., de Haan, J. F., Kleipool, Q., van Weele, M., Hasekamp, O., Hoogeveen, R., Landgraf, J., Snel, R., Tol, P., Ingmann, P., Voors, R., Kruizinga, B., Vink, R., Visser, H., and Levelt, P. F.: TROPOMI on the ESA Sentinel-5 Precursor: A GMES mission for global observations of the atmospheric composition for climate, air quality and ozone layer applications, Remote Sensing of Environment, 120, 70–83, https://doi.org/10.1016/j.rse.2011.09.027, 2012.