

# Interactive comment on "Comparison of TROPOMI/Sentinel 5 Precursor NO<sub>2</sub> observations with ground-based measurements in Helsinki" by Iolanda Ialongo et al.

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I read the article of lalongo et al., discussing comparisons of S5p TROPOMI NO2 with ground-based data, with great interest. Given the significance of S5p TROPOMI NO2 for air quality assessments across the globe, its validation is clearly of great importance. I recommend publication in AMT with minor revisions.

## Overall.

1/ There are indicators for bias (the MD and MRD) but not for the dispersion of differences, for example the standard deviation of the differences or the interquartile range

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of the differences. Please add e.g., the standard deviation of the differences to the methodology, together with the definitions for MD and MRD, and discuss the results in the manuscript, including table 1 and 2.

2/ Although the uncertainties of S5p NO2 (p. 4) and Pandora (p. 5) are shortly mentioned, it is not discussed (e.g., in the conclusions) whether discrepancies between S5p and Pandonia are reasonable with respect to the uncertainties. Both S5p NO2 and Pandora measurements have an uncertainty provided per measurement. In the time series of co-located points of S5p NO2 and Pandora, the error bars based on the provided uncertainties can be added. It can then also be discussed whether the S5p values based on the CAMS a-priori are meaningfully different from the TM5-MP based S5p values.

3/ Minor comment: be consistent in the units for NO2 column number density, and preferably use  $10^{15}$  molec cm<sup>-2</sup> as unit in the Tables and figures, as this is very commonly used in NO2 column comparisons. Currently the authors use  $10^{14}$  molec cm<sup>-2</sup> in table 1 and 2, and  $10^{16}$  molec cm<sup>-2</sup> in e.g., Fig. 5.

# **Detailed comments**

Abstract, line 5. 'TROPOMI total columns underestimate ground-based observations for relatively large Pandora NO2 total columns'. It should be added here that TROPOMI overestimates for the lower columns. Also the obtained bias (absolute scale and relative), and the dispersion of the differences (e.g., the standard deviation of differences, as noted above) should be added in the abstract.

Abstract, line 9. Here it is stated that "Replacing the coarse a-priori NO2 profiles with high-resolution profiles from the CAMS chemical transport model improves the agreement between TROPOMI and Pandora total columns for episodes of NO2 enhancement." Please add a statement on the overall agreement and/or episodes of low NO2.

Introduction. p. 2, around line 27. Here, the authors should add that there is an operational validation of S5p products by the S5P-MPC-VDAF (S5P - Mission Performance Center - Validation Analysis Facility, http://mpc-vdaf.tropomi.eu/) which includes online comparisons and validation reports using the S5p total NO2 vs Pandora from the Pandonia Global Network, including the one at the Helsinki site.

p. 4, line 4. I would add here that the summed total column is the one that is recommended by the data provider.

p. 4, line 27 and following. More detail should be provided here:

- Is reanalysis data used ?
- make clear that CAMS global, despite the name similarity, is a very different model compared to CAMS regional
- add reference for CAMS global, the horizontal resolution, and the vertical range.
- 'better description of free troposphere': do you mean better compared to TM5-MP
  ?
- make more clear that you are actually constructing a hybrid profile from CAMS regional and CAMS global.
- line 29. '...using the CAMS (...) a-priori profiles'. Certainly this first time, I suggest to formulate instead 'using the hybrid CAMS regional/CAMS global a-priori profiles (called shorthand "CAMS a-priori profile" from now on) ' or some similar formulation.
- line 30. 'These ratios were available on the regular CAMS 0.1x0.1 grid' This sounds as if the authors obtained the AMF ratios from elsewhere. But if I understood well, you actually calculated the ratios yourself, using input from the hybrid CAMS regional/CAMS global profile and from the S5p product, right? Also, the

procedure how to calculate the AMF ratio using CAMS a priori data and S5p NO2 input (averaging kernel, TM5-based AMF) should be explained. E.g., likely there was need for (i) a vertical regridding of the CAMS profile to match the vertical grid of the averaging kernel of S5p NO2, and (ii) an horizontal interpolation (if so, what kind of interpolation) of the CAMS global profile to the CAMS regional grid.

These details can be discussed here, or alternatively in an appendix or the supplement.

p. 6, line 20. 'Pandora retrievals with data quality flag value of 0, 1, 10 or 11'. Pandora measurements can occasionally become negative and even reach several Pmolec cm-2 in the negative. This is drastically reduced when only focusing on high-quality data with 0, 10 flags. Was there any filtering on negative Pandora values, or were these averaged together with the positive values, or were these -by chance- no longer present after co-location with TROPOMI?

p. 7, fig. 2. I share the concerns of reviewer 1 on the clarity of this figure.

p. 7, line 5. 'CAMS a priori summed column' is somewhat ambiguous. A reader could assume this is a column purely derived from CAMS information. I suggest: 'the newly derived summed column, using the CAMS a-priori profile,...,is calculated as...'

p. 7, line 2. 'ratio (R) between the tropospheric column retrievals...' This is unclear. From section 2.1, I assume R is the ratio of the original  $AMF_{trop}$  of the S5p NO2 product and the newly calculated  $AMF_{trop}$ .

p. 7, Eq (3). From the formula, it is clear that the stratospheric contribution is not updated (still based on TM5-MP), while CAMS global is nonetheless available (as the authors used it for the free troposphere). A motivation is needed why CAMS regional+global is used for the troposphere while TM5 is kept for the stratosphere.

p. 9, Table 1.

· Regarding the slope from orthogonal regression, it should be noted in the text

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that this technique assumes that the standard deviation from random error in y (S5p NO2 total column) and x (Pandora total column) are equal, which is not at all guaranteed. See e.g., Carroll (1996), with  $\eta$  of Eq (4) assumed 1, or Wu (2018), who do not recommend orthogonal distance regression.

• What is the meaning of the number after the  $\pm$  ? Is it the standard deviation of the mean? This should be explained in the table footnote. Similar for Table 2.

p. 10, line 19. What is the impact of changing the co-location criteria (spatial and temporal) on the standard deviation of the differences and the correlation coefficient?

p. 10, line 23. What is meant by 'variability' here? The amount by which the MD changes?

p. 12, Fig. 5 right panel. Add error bars (based on the provided uncertainties) to S5p NO2 and Pandonia points. This figure will be clearer when using points instead of lines.

p. 12, Fig. 6. What is the meaning of the vertical error bars? The standard deviation of the values in the month? This should be explained in the caption.

p. 12-13 ( about the evaluation of the effect of using CAMS a-priori profiles) + Fig. S3

- Please add in Fig. S3 error bars on the S5p NO2 TM5-MP points and on the Pandonia points. This will give an indication whether the update with the CAMS a-priori profiles is significant with respect to the uncertainties.
- Assumed that the numbers after the  $\pm$  in Table 2 are standard deviations of the mean, it seems to me that the difference between the MD calculated with TM5-MP profiles on the one hand, and the MD calculated with CAMS a-priori on the other hand, is not statistically significant. Same remark for the MRD. This should then be also reflected in the abstract and the conclusions.

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p. 13 line 4-5. 'On the other hand, in cases of low concentrations, where TROPOMI tends to overestimate the VCDs compared to Pandora, the use of CAMS a-priori profiles slightly worsens the agreement with Pandora by increasing the positive bias. ' Looking at Fig S3 this effect seems really small to me and is probably not statistically significant. Add in Table 2 entries for 'Pandora high' and 'Pandora low' so one can conclude what is the significance of this effect.

p. 13, Conclusions. Here, it should also be stated whether the S5p vs Pandora discrepancies are reasonable (or not) in light of the measurement uncertainties of S5p and Pandora.

p. 13, line 22. 'while low values are overestimated' A short discussion on the possible reasons should go here. Does this mean that TROPOMI has a positive systematic error at low NO2 values? Or that the Pandora instrument has a negative systematic error? Or is it somehow due to the still relatively coarse resolution of S5p NO2? And is the overestimation actually significant with respect to the uncertainties?

p. 15, Data availability. It should be noted that there is no general open access to the S5p Expert users Data Hub, only to the S5p Pre-Operations Data Hub. Also, the point of access for CAMS regional and CAMS global should added here, and exactly which kind of data was used (forecast, reanalysis?).

## References

Carroll, R. J. and Ruppert, D. The Use and Misuse of Orthogonal Regression in Linear Errors-in-Variables Models The American Statistician, 1, feb 1996, 50

Wu, C. and Yu, J. Z. Evaluation of linear regression techniques for atmospheric applications: the importance of appropriate weighting Atmos. Meas. Tech., 2, 2018, 11, 1233-1250

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