

Interactive comment on “Sulfur dioxide retrievals from TROPOMI onboard Sentinel-5 Precursor: Algorithm Theoretical Basis” by N. Theys et al.

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Replies to the reviewers comments are below in italic; changes in the text are in blue in the revised version of the manuscript.

Reply: The authors gratefully thank all the reviewers for their thorough review and interesting comments which contributed to improve the manuscript. Review of anonymous Referee #1 This paper introduces the SO₂ retrieval algorithm for the upcoming S-5P TROPOMI instrument. In addition to a description of the product requirement and retrieval algorithm (wavelength calibration, fitting window selection, DOAS analysis, bias correction, AMF calculation), the authors also provided a list of potential error sources in the retrievals and gave estimates of these errors where possible. Results from comparison with a verification algorithm (also based on the DOAS technique) were given,

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showing generally good agreement for a few volcanic cases, although the agreement between the two algorithms seem to be worse for higher SO₂ loading. The authors also discussed future effort and potential data sources for product validation. Overall, this is a well-written and well-organized paper on an important product from the TROPOMI mission. The authors' effort in characterizing retrieval errors, while done in the absence of actual data before the launch of the instrument, is appreciated. I would recommend that the paper be accepted for publication in AMT after some minor changes suggested below. Page 2, line 21: another recent paper on long-term trend of SO₂ is He et al., 2016: He, H., Vinnikov, K. Y., Li, C., Krotkov, N. A., Jongeward, A. R., Li, Z., Stehr, J. W., Hains, J. C. and Dickerson, R. R. (2016), Response of SO₂ and particulate air pollution to local and regional emission controls: A case study in Maryland. *Earth's Future*, 4: 94–109. doi:10.1002/2015EF000330.

Reply: changed in the text.

Page 4, Line 6: consider spelling out the acronyms for the first use (e.g., CAPACITY and CAMELOT). A list of acronyms in the appendix may also help the readers.

Reply: changed in the text. A list of acronyms has been added in Annex.

Page 5, Line 23: special should be spatial?

Reply: changed in the text.

Page 8, Line 12, maybe refer readers to Table A3 so that it is easier to find out which L2 cloud product will be used?

Reply: changed in the text.

Page 9, Line 16: change “enables to define” to “enables us to define” or “enables defining”.

Reply: changed in the text.

Page 13, Line 27: “prior to the” DOAS “analysis”?

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Reply: yes, changed in the text.

Page 14, Line 13: the average residual is calculated for the entire row or orbit? Also what is the percentage of pixels rejected in OMI?

Reply: we believe there is a misunderstanding. The word "pixel" refers to "detector pixel". The spike removal scheme applies on wavelength dimension not on across-track or along-track dimensions. For OMI, only few wavelengths are discarded from the DOAS analysis (maintaining largely the inverse problem as over-constrained) for OMI observations mostly in the South Atlantic region. We have clarified the text.

Page 15, Line 22: typically how many pixels are available for averaging in each slant O3 column bin?

Reply: not all O3 bins are populated equally but the number of pixels varies in the range of 3×10^3 - 3×10^4 per across-track position and for 2 weeks moving averages. For TROPOMI, we expect double more pixels. We propose not to report those numbers in the text as they are not essential for the understanding of the method.

Page 20, Line 16: "what is the SO2 vertical profile" should be "what the SO2 vertical profile is".

Reply: changed in the text.

Page 20, Line 24: so both fixed profiles and TM5 profiles will be used in the operational retrievals?

Reply: yes, we have made it clearer in the text.

Page 21, Line 9: please specify how rescaling will be done.

Reply: we have added the following sentence: The TM5 SO2 profile is shifted to start at ps and scaled so that volume mixing ratios are preserved (see Zhou et al., 2009).

Page 21, Line 12: if TM5 SO2 profile will be used, why not also use its temperature

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profile (instead of assuming a constant lapse rate everywhere).

Reply: it could be done but the impact on the AMF will be very small.

Page 23, eq. 12: define m'

Reply: m' is the weighting function. We have clarified the text.

Page 24, Line 22: is it implied that a constant 0.2 DU positive bias exists in the slant column SO2?

Reply: no, on average the bias is zero but in some places, SCDs might be biased (low or high) by max 0.2 DU (in absolute value).

Page 26, Line 28: how was this uncertainty estimated?

Reply: It has been estimated from averaged background corrected SCDs over clean regions (e.g. deserts). It has been clarified in the text.

Page 27, Line 6: do you expect uncertainty in LIDORT in terms of comparison with VLIDORT or TOMRAD?

Reply: We have not compared LIDORT with VLIDORT or TOMRAD but we expect relatively small error contribution from RTM (see also Error source # 12, section 3.2.2).

Page 31, Line 22: "error associated" should be "associated error".

Reply: changed in the text.

Page 40, Line 6: "newly" should be "new"?

Reply: changed in the text.

Page 42, Line 14: does the comparison between the two algorithms suggest that the measurement requirements will be met?

Reply: yes, this is true. It is also mentioned in Table 1 that requirements for volcanic SO2 will be met for $VCD > 0.5$ DU. We have added a reference to section 4 (on verifica-

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tion results) in the section 2.1 on product requirements.

Table 6, #19: is 15% an upper limit for the effects of anthropogenic aerosols on air mass factor? Could this be an underestimate given the uncertainties in aerosol properties and vertical distribution?

Reply: we agree with the referee. Clearly the uncertainties due to aerosols can be much larger than 15% because of uncertainties on aerosol properties and vertical distribution (as mentioned on page 31). In table 6, we intended to simply report on published estimates but apparently there is a risk that the reader over-interprets the numbers and we propose to write 15% as an approximate value and not as an upper limit as it is now.

Figure 11: I'm not sure that the figure is completely necessary: this is essentially the same program implemented in different systems and the results are expected to be very close if not identical.

Reply: the SO₂ prototype algorithm has not been provided to the operational team as a plug-and-play software package and the operation team had to rewrite most of the algorithmic modules. It required a lot of work and technical verification which is summarized in Fig 11. Although it is true that the figure is not essential, we think it also does not hurt to have a summarizing figure to illustrate the complete implementation of the algorithm in the operational environment.

Review of anonymous Referee #2

- General Comments

This manuscript describes the SO₂ retrieval algorithm of TROPOMI onboard Sentinel-5P. It well summarized the current status of the SO₂ retrieval techniques, requirements, its error estimates, and validations. The retrieval strategy looks well-planned and this manuscript would be important for the future users of TROPOMI. Hence I would recommend publication of this manuscript for AMT after minor revisions below.

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- Specific Comments Page 18, lines 12-17 : The surface reflectance from Kleipool et al. (2008) generally provides reliable information, but there might be the better option for TROPOMI which has better spatial resolution (which is important for small urban and point source areas). At least discussion related to the spatial resolution of the surface reflectance and alternatives for the database would be helpful for this moment of ATBD.
Reply: clearly, other surface reflectance databases more appropriate for S5P will become available and will be considered in next algorithmic versions. We have added a paragraph on this in the text. Page 25, lines 23-27 and Page 26, lines 11-14 : The measurement accuracy/uncertainty is major error source of SO₂ retrieval with its measurement sensitivity as the author stated. Thus, it is valuable to add more details of the predicted measurement uncertainties. It might be challenging to evaluate/anticipate the measurement errors at this moment, but at least the authors could add brief discussion based on the requirements of L1b measurement and prior missions so that how much improvements would be expected. The radiometric calibration might include spectrally high-frequency errors such as the stray light and polarization sensitivity (particularly for window 1, from 312 to 326 nm). This might be included in Error source 8, but I would recommend to list those specifically since they are known high-frequency error sources.

Reply: We understand the concern of the reviewer and we agree that evaluating these measurement errors is challenging at the moment. Once the instrument will be operating, it will certainly be an important task to characterize instrumental-related spectral features, assess whether they interfere with SO₂ retrievals and correct for those (either as part of L1b processor or in the form of pseudo absorption cross-sections in the DOAS analysis). We have added the following lines in Error source 8: Unknown or untreated instrumental characteristics such as stray light and polarization sensitivity can introduce spectral features that may lead to bias in the retrieved slant column data. To certain extend these can be prevented by the DOAS polynomial and the intensity offset correction settings, as long as the perturbing signals are a smooth function of wavelength. Conversely, high-frequency spectral structures can have potentially a

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large impact on SO₂ retrievals depending on their amplitude and whether they interfere with SO₂ absorption structures. At the time of writing, it is hard to evaluate these measurement errors. Once the instrument will be operating, such measurement errors will be characterized and correct for, either as part of L1b processor or in the form of pseudo absorption cross-sections in the DOAS analysis.

- Technical corrections Page 17, line 16 and Page 19, line 8 : Please check if the A_c is defined in the manuscript. Please clarify the definition of f_c and f_{eff} which are used for “effective cloud fraction”.

Reply: We have defined A_c and clarify the text when needed.

Page 23, line 14 : I would recommend to use different symbol for error to distinguish from the absorption cross section.

Reply: we prefer to keep these symbols because they were adopted in other S5P ATBDs. Moreover, in this section, it is clear they are not referring to absorption cross-sections.

Please also note the supplement to this comment:

<http://www.atmos-meas-tech-discuss.net/amt-2016-309/amt-2016-309-AC1-supplement.pdf>

Interactive comment on Atmos. Meas. Tech. Discuss., doi:10.5194/amt-2016-309, 2016.