

Reply to Comment on egusphere-2025-5836 by Anonymous Referee #2

Referee comment on "Improved NO₂ spectral fits for TROPOMI and OMI by removing wavelengths around 430 nm" by Jos van Geffen et al., <https://doi.org/10.5194/egusphere-2025-5836-RC2>

⇒ The referee report is copied below; the reply is preceded by an arrow, like this text.

Apart from the changes resulting from the review process, we have carried out the following updates, which do not affect the conclusions of the paper:

- TROPOMI processor v2.9.1, which includes the "NO₂-gap approach" of the paper, was activated on 22 November 2025; the text has been updated to represent this fact where appropriate.
 - Since we now have a few months of v2.9.1 data, a quick comparison of results before and after the switch is added at the end of Sect. 4.2
 - Fig. 2 in Sect. 2.2.2 is extended to include the year 2025; the figure caption was reformulated to improve readability.
 - Fig. A1 in App. A is extended to contain the full year 2025.
 - Meanwhile the OMI collection 4 NO₂ slant column data, named OMNO2A, are released by NASA; the URL of the download access is added to the "Data availability" section. NASA has assigned a DOI to both the dataset and the ATBD: <https://doi.org/10.5067/AURA/OMI/DATA2433>. Unfortunately, this DOI appears not yet activated; it should likely lead to a landing page such as the one for the collection 4 cloud data (OMCLDO2): <https://doi.org/10.5067/AURA/OMI/DATA2407>. Hopefully, NASA has activated the OMNO2A DOI by the time the paper is published.
 - A few minor textual corrections were carried out.
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General comments

This manuscript presents a detailed investigation of the NO₂ slant column fitting results from TROPOMI and OMI. Fitting residuals are carefully inspected showing that spectral misfits are systematically encountered around 430 nm, i.e. approximately in the middle of the retrieval range used for operational NO₂ retrieval from both satellite sensors. These misfits are mostly observed above open water scenes (primarily Pacific, Atlantic and Indian oceans) and are attributed to the combined effect of inaccurate corrections for rotational Raman scattering (RRS) in air and vibrational Raman scattering (VRS) in water, the latter effect being ignored in the retrieval settings due to its complexity.

The authors present a convincing quantitative analysis of the dependency of the fit residuals on various parameters which clearly shows that the discrepancy is systematic and observed mainly above the water in a similar way for OMI and TROPOMI. This reinforces the interpretation of the nature of the problem. To solve the issue, they propose to introduce a 5-nm gap (428-433 nm) in the spectral range used for NO₂ retrieval. The introduction of this gap is shown to reduce fitting RMS and SCD errors by about 10% while the NO₂ SCD is seen to decrease by a few percent over oceans. Overall, the proposed algorithm adaptation only affects the retrieved NO₂ columns by a few $\mu\text{mol}/\text{m}^2$ (equivalent to a few 10^{14} molec/cm²) and is therefore essentially cosmetic.

⇒ We thank the referee for these kind words.

Though the overall impact of the adaptation is not large in terms of numbers or percentages, it is in the end quite an important improvement, evidenced by the 10After all, we are at a stage where improvements in the NO₂ retrieval with large impact have been well studied, so that further improvements will be smaller and smaller in magnitude.

The manuscript is well written and organized, and figures are all clear. The scientific approach to characterize fitting residuals and their variations is sound and appropriate. However, I remain unconvinced by the approach chosen to resolve the issue. In my view, especially considering the discussion in section 6.2, the intensity offset correction seems to provide an equally good correction while conserving the full spectral information.

⇒ As we argue in Sect. 6.2 the IOC indeed gives similar results at the NO₂-gap approach, but the IOC will still introduce artifacts because (a) it has a narrower peak around 430 nm than the

problem seen in the residual, (b) the (solar) reference spectrum has structures outside that peak which affect the retrieval as well, and (c) the physical interpretation of the intensity offset term is unclear. These three issues are avoided by the NO₂-gap approach.

Another possible approach could have been to perform a PCA analysis of the spectral residuals over oceans and use it to generate an additional pseudo cross-section accounting for the misfit. Similar approaches have been recently exploited with success in correcting other misfit problems (e.g. the impact of scene inhomogeneities affecting the effective instrumental response function at the edge of bright scenes).

⇒ A principle component analysis (PCA) is indeed another option for NO₂ retrieval, and it has been done by some groups but it is not a common practice for the groups involved in the TROPOMI and OMI retrieval. PCA should then, however, be applied to the reflectance spectrum, not on the spectral residual, as the shape of the spectral residual is determined by the fit results, i.e. by, for example, an incorrect NO₂ column value.

In a retrieval such as ours, we prescribe a selected set of physical quantities we know are involved, though we at the same time know that we do not actually include all quantities that are involved, simply because we do not know all in detail and because reference spectra of different components may not be fully independent (orthogonal).

Given the nature of the paper, we consider a discussion of these points beyond the scope of the paper.

In the end, the main benefit of the change in algorithm is to provide more realistic estimates of the random uncertainties in the retrieved slant columns. This aspect could be better stressed in the conclusions of the study.

⇒ The wording in the 5th paragraph of Sect. 7 has been expanded a little in the light of this remark.

That said, this article is of high quality and interesting in many respects, and it should certainly be published in AMT, once the comments below have been considered.

Detailed comments

Pg. 1, line 8 and pg. 2, line 23

The authors repeatedly state that VRS cannot be corrected by way of a scalable reference spectrum, however it is not clear why it is so. References given for other VRS studies show that corrections can be implemented in some cases. Please make it clear in which way the correction that would be needed for NO₂ is different from what has been successfully applied in other studies.

⇒ The argument is given on page 2, at the line you mention, as well as in the last section: the effect of VRS depends on the viewing geometry and conditions of the water and each situation would thus require its own reference spectrum and thus on-the-fly radiative calculations, which is not an option for operational world-wide processing. The 2nd paragraph in Sect. 7 has been updated.

Pg. 3, line 17

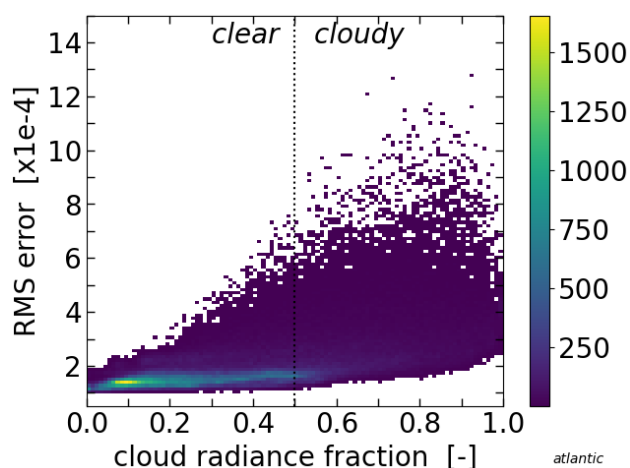
As written, this sentence sounds a bit weird. I would suggest: "The Tropospheric Monitoring Instrument, sole payload aboard ESA's Sentinel-5 Precursor (S5P) spacecraft, was launched on 13 October 2017 into an..."

⇒ Thank you for this suggestion, the text has been updated accordingly. The first sentence of Sect. 2.1.2 on OMI has been changed in the same way.

Pg. 5, line 20

The Ring vector was calculated using the Dobber et al. atlas. Have you checked the potential impact of using another (more recent) solar reference spectrum for the calculation of the Ring cross-section (e.g. TSIS-1, or Chance and Kurucz)?

⇒ No, we have not investigated other solar reference spectra. But even with another solar reference, there will be only a single Ring reference, i.e. with a fixed peak at 430 nm, which thus will still not reflect the variation of the Fraunhofer lines with the solar activity cycle. From the general point of view of TROPOMI retrievals, the possible use of the TSIS reference will be investigated,



Fig_RC 1: Scatter plot of the RMS error as function of the cloud radiance fraction for the Atlantic Ocean section.

and likely before the next update (scheduled in Nov. 2026 to v3.0.0 and in preparation for the full mission reprocessing).

Pg. 11, line 19

Here, I would expect the RMS to be smaller over cloudy pixels, due to the increased S/N ratio over bright scenes (more photons being reflected to the satellite). Maybe the reason for the low RMS_430 ratio is simply that water is hidden by clouds. Please clarify.

⇒ Fig_RC 1 shows the RMS error as function of the cloud radiance fraction for the Atlantic Ocean section of Sect. 3.1: although there is indeed more light over cloudy scenes (and thus the SNR is higher there), the fit residual is (much) more noisy over cloudy scenes. The text at the end of Sect. 3.1 has been updated to mention this.

Pg. 27, line 16

I follow the reasoning here, but the residual plot in Fig.17 still does show an almost complete compensation. As mentioned later in the text, the broad-band structures visible in the fit residual themselves do not represent the missing reference spectrum, because the shape of the residual is the result of DOAS adjusting all fit parameters so as to minimise the residual. Therefore, although the peak at 430 nm is narrower than found in the residuals, it might well be that the IOC compensates well for the effect over the full interval.

⇒ As mentioned above in the General Comments, the IOC does indeed give similar results, but we are afraid that the IOC may introduce additional features in the fit, because it has a structure outside the peak, while the NO₂-gap approach seems a more physically sound approach because it is simply a matter of (re)defining the fit window limits to the optimal range(s).

Section 4.2, table 4

In my understanding, the main benefit of the NO₂-gap is to improve residuals and therefore to bring the SCD errors closer to the statistical noise. It would be interesting to further discuss this point and maybe add values in table 4 showing how close the resulting SCD errors are to statistical errors.

⇒ Improving the fit residuals, in terms of reducing the DOAS SCD uncertainty estimate and the RMS error, is indeed the objective. But this does not necessarily mean that the DOAS and statistical uncertainty will lie closer together: how close these are together also depends on the accuracy of the statistical uncertainty.

Whether the two uncertainties are closer together or not due to the NO₂-gap approach can in principle be seen from the numbers in Table 4.

– For the clear-sky case the DOAS uncertainty changes by a factor of about 0.95, while the statistical uncertainty remains almost unchanged (factor 0.99), so that for this case the two uncertainties have come somewhat closer together.

– For the cloudy case, however, the two have gone further apart: the DOAS uncertainty has changed a little (factor 0.98) while the statistical uncertainty has been improved by a factor of 0.91.

The important conclusion is that the NO₂-gap approach either reduces the uncertainties or leaves them more or less unaffected, without deteriorating the results. The text of Sect. 4.2 has been modified a little.

Section 6.1

I understand that the spectral features over Tibetan lakes are related to a different mechanism, than those found more generally over oceans. Their impact on the NO₂ SCDs is also more significant. It is not fully clear from the text whether the "NO₂-gap" approach is able to reduce the observed bias on the NO₂ SCDs. Please clarify.

⇒ As mentioned at the end of Sect. 6.1 the effect of the NO₂-gap approach on the GCD values is minimal, so no: the approach does not solve the observed bias, though the fit quality is improved (lower SCD and RMS error). To solve the bias, we need to know the characteristics of the dissolved matter. The end of Sect. 6.1 has been expanded somewhat to express this.

Spelling, typos

Pg. 3, line 4 – Remove the 's' at the end of 'shows' in "Residuals may also shows broad-band.."

Pg. 7, line 7 – Replace 'encounted' by 'encountered'

Pg. 19, line 8 – Replace "where" by "were"

Pg. 24, line 33 – Replace "deaper" by "deeper"

⇒ Thanks for spotting these typos – they have been corrected.