Title: Retrieval of SO₂ columns from FY3F/OMS instrument observations

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Thomas Visarius

We thank the AMT Editors and the anonymous Referees #1 and #2 for handling the review process, carefully reading our manuscript, and providing constructive comments. The paper was corrected according to the suggestions of the two reviewers. We hope that in dealing with the comments put forward by Anonymous Referees #1 and #2, the quality of the manuscript was improved. We addressed the comments below.

Answer to Referee #1

1. Reviewer 1: Treatment of missing retrieval data. It is understandable that the test retrievals can fail to produce valid data in certain circumstances for certain areas. However, I find the treatment of this missing data in the manuscript to be rather odd. The authors take great care to document the technical nature of missing data in retrieval output (e.g. they explicitly state how "nan values" and fill values are represented in color maps), which I do not believe to be relevant in a scientific publication. However, in most cases they do not explain why this data is missing, which would be highly relevant, and often essential. These explanations should be added.

Authors: We thank the reviewer for this valuable comment. We agree that, in addition to describing how missing values are represented in the figures, it is important to explain the reasons for missing retrieval data. In the revised manuscript, we have added explanations for the main causes of missing data in the retrieval results, such as the gap between two orbits, Nan values in the downloaded TROPOMI data, and invalid DOAS fitting results.

The following changes were made in the revised manuscript:

1) P15, L302: For the Nan values in the TROPOMI COBRA data, we contacted one of the developers of the COBRA algorithm, Dr. Nicolas Theys, to determine their origin. The TROPOMI COBRA L3 grid product (0.022° × 0.022° equal latitude–longitude grid) was generated from L2 data using the HARP gridding tool with a Quality Assurance (QA) filter (QA > 0.5) to remove low-quality data.

In Section 4, at the end of the second paragraph, we added the following sentence to explain the cause of Nan values in the TROPOMI COBRA data: "The quality filtering leads to some gaps in the COBRA data."

2) In Figure 8, revised "The missing pixels in the Figure c are caused by Nan values in TROPOMI COBRA data" to "The missing pixels in Figure c are due to quality filtering applied to TROPOMI COBRA data" to clarify the cause of the missing pixels.

In Figure 9, revised "The missing pixels in the Figures b and c are caused by the gap between the two orbits and the Nan values in TROPOMI COBRA data" to "The missing pixels in Figure b are due to the gap between the two TROPOMI orbits, while those in Figure c are due to the quality filtering applied in the TROPOMI COBRA data" to more clearly explain the causes of the missing pixels in each subfigure.

In addition, similar descriptions of missing data in TROPOMI COBRA data have been modified throughout the manuscript.

2. Reviewer 1: Lack of summary/conclusions of agreement between OMS and TROPOMI. I would have liked to see more clear statements and a summary regarding agreement of OMS and TROPOMI data. The authors provide quite a few possible reasons for differences in SO₂ column values, but do they generally believe that those reasons are sufficient to explain the differences? How do these differences compare to OMS and TROPOMI error estimates? Also, although error

analysis was discussed in detail, a clear representation and discussion of the resulting error values seems to be missing.

Authors: We thank the reviewer for this comment. We agree that the manuscript would benefit from a clearer summary of the agreement between OMS and TROPOMI SO₂ products. Our responses to these suggested revisions are provided below.

1) **Comment:** I would have liked to see more clear statements and a summary regarding agreement of OMS and TROPOMI data.

Answer: In the revised manuscript, the first paragraph of Section 6 has been reorganized into four paragraphs, with expanded descriptions that more clearly elaborate on both the agreement and the differences between the OMS and TROPOMI results. The revised content in the revised manuscript is as follows (in red font):

This study utilized TOA reflected radiance data from the Chinese FY3F/OMS-N instrument, launched in August 2023, to retrieve global SO₂ columns with a DOAS approach. Based on the characteristics of the OMS instrument and the performance of its L1 data, specific schemes, including solar spectrum selection, spectral soft calibration, and background offset correction, were developed to effectively reduce along-track stripes and across-track asymmetry in the initial OMS SO₂ retrievals.

The OMS SO₂ retrievals were compared with TROPOMI DOAS and TROPOMI COBRA SO₂ products in clean oceanic regions, under volcanic eruption conditions, and in anthropogenic emission regions. The comparison results indicate that OMS retrievals show reasonable agreement with TROPOMI products, have good stability in clean oceanic regions and can be used to monitor SO₂ emissions from volcanic eruptions and anthropogenic sources. In selected clean oceanic regions, the SO₂ values of both OMS and

TROPOMI follow approximately a normal distribution centered around 0, with most values concentrated between -2 DU and 2 DU. For the Sundhnúkur and Nyamuragira volcanic eruptions, FY3F/OMS SO₂ retrievals successfully capture the spatial distribution and high-concentration plumes of volcanic SO₂, similar to the TROPOMI DOAS and TROPOMI COBRA 7 km SO₂ results. Over the Sundhnúkur volcano, OMS and TROPOMI DOAS show a high correlation of ~0.87, and OMS and TROPOMI COBRA reach ~0.76, indicating good overall agreement. However, OMS tends to underestimate SO₂ at high columns (>50 DU) due to saturation in the 312–326 nm fitting window. In anthropogenic emission regions, OMS and TROPOMI SO₂ products show generally good consistency in detecting anthropogenic SO₂ emissions, with correlation coefficients ranging from about 0.5–0.6 over the Persian Gulf and up to 0.91–0.93 over Norilsk.

The differences between OMS and TROPOMI SO₂ results may be related to differences in local overpass times, spatial resolution, observation angles, and the L1 and L2 processing algorithms (e.g., differences in L1 radiometric and spectral calibration methods, SO₂ retrieval fitting windows, AMF strategies). Among these, the AMF used in the SO₂ column retrieval is a major contributor to the differences between OMS and TROPOMI SO₂ results. For example, in the case of the Sundhnúkur volcano, the lack of accurate information on the vertical SO₂ profile can lead to discrepancies of more than a factor of two when comparing the OMS and TROPOMI SO₂ results. Random noise and uncertainties from background correction are relevant for low SO₂ scenarios, such as over the Persian Gulf, and lead to scatter in the order of several DU. However, the results for Norilsk demonstrate that under relatively constant emission conditions, good agreement can be achieved with a simple AMF when the satellite overpass times are well matched.

In summary, the agreement between the OMS and TROPOMI measurements is within expectations, taking into account the differences in

satellite overpass times and the uncertainties associated with AMF assumptions. With its high spectral and spatial resolution, morning overpass time, daily global coverage, and reliable SO₂ retrieval results, OMS will provide effective data support for monitoring the continuous SO₂ changes from global volcanic eruptions and anthropogenic activities, helping to fill the spatial and temporal gaps in the existing global satellite network.

2) **Comment:** The authors provide quite a few possible reasons for differences in SO₂ column values, but do they generally believe that those reasons are sufficient to explain the differences?

Answer: Although several possible reasons for the differences in SO₂ column values have been listed, we are not fully confident that these explanations are sufficient to account for all observed discrepancies. There may also be factors beyond our current understanding. At present, we thought that the reasons listed can explain the observed differences, and that the observed differences are in the expected order of magnitude.

3) **Comment:** How do these differences compare to OMS and TROPOMI error estimates?

Answer: Some of the error sources of OMS and TROPOMI SO₂ retrievals overlap with the factors causing differences between the two products. For example, errors in L1 radiometric and spectral calibration are not only error sources that affect the accuracy of both OMS and TROPOMI SO₂ retrievals, but also contribute to the differences between them. Similarly, the choice of retrieval window is both an error source for product accuracy and a factor leading to differences between OMS and TROPOMI SO₂ retrievals.

Some factors contributing to the differences are not intrinsic error sources of the OMS and TROPOMI SO₂ retrievals. For instance, the difference in local overpass times and spatial resolution will inevitably lead to discrepancies, as

the instantaneous atmospheric states observed by OMS and TROPOMI are not the same.

4) **Comment:** Also, although error analysis was discussed in detail, a clear representation and discussion of the resulting error values seems to be missing.

Answer: Thank the reviewer for this valuable comment.

There are many factors that affect the accuracy of SO₂ retrievals. In principle, one should analyze how each individual error source contributes to the total retrieval uncertainty. In practice, however, these error sources are complex and difficult to separate. For example, instrument random noise and calibration errors are challenging to quantify precisely since the true SO₂ values are not known. Although the official OMS L1 product provides specified performance requirements, our in-orbit tests indicate that the actual OMS L1 errors deviate from the planned specifications for certain parameters. At present, it is therefore difficult to obtain precise quantitative estimates of how instrument noise contributes to the SO₂ retrieval accuracy.

In addition, to address striping and cross-track asymmetry in the SO₂ SCD retrievals, we applied a background offset correction scheme. However, since the true SO₂ values are unknown, it is not possible to fully verify the accuracy of these corrections. While values over clean regions and their scatter could be used as an indicator of the correction quality, this method does not account for possible overcorrections or systematic biases.

Taking the OMS 20240823_1036 orbit as an example, here we present two plots of the SO₂ SCD retrieval RMSE and spectral fitting error (SFE). These figures show the magnitude and distribution of errors in the retrieved SCDs. Both RMSE and SFE values remain relatively large, with pronounced striping features, and are particularly high on the right side of the orbit. This is most likely related to instrument radiometric and spectral calibration errors, which are difficult to separate and remain a major source of uncertainty. The

corrections applied in our product largely reduce the impact on the SO₂ columns, but proper accounting for this in the error estimates is difficult. Ongoing improvements to the OMS L1 data are expected to reduce striping and asymmetry in the calibration in order to improve SO₂ retrieval accuracy. Considering these aspects, we decided not to include the RMSE and SFE results in this revised manuscript.

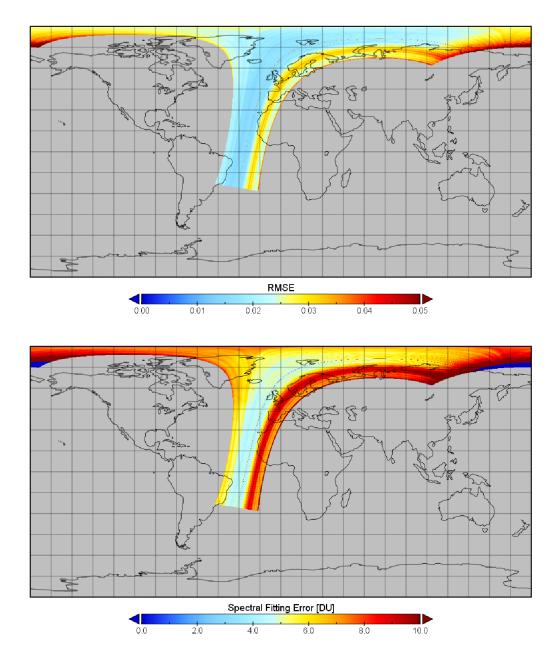


Figure: RMSE and Spectral Fitting Error of OMS SO₂ SCDs for OMS orbit 20240823_1036.

In response to Reviewer 2's comment, we have supplemented the AMF section (P35, L593-603) with additional calculation results to provide a rough estimate of the errors introduced by the simplified AMF strategy. The added contents are shown in red font below.

Neglecting forward model errors, Figure 22 shows the dependence of AMF on SZA, VZA, AS, wavelength, O₃ column, and SO₂ profiles. The AMFs were calculated with SCIATRAN Box-AMFs using six assumed SO₂ profiles. Here six SO₂ profiles were constructed, representing clean conditions, low, medium, and high anthropogenic SO₂ emissions, volcanic degassing with plume heights around 2 km, and volcanic eruptions with plume heights around 6 km. As shown in Fig. 22, although AMF values are generally close to 1 under typical atmospheric and surface conditions (non-ice/snow-covered), the magnitude of biases introduced by the simplified AMF approach (AMF=1 for clean regions and non-ice/snowcovered areas, while the other is AMF=2 for the ice/snow-covered areas) varies significantly with different conditions. Surface albedo is the major factor affecting AMF accuracy. For instance, AMFs can differ by up to a factor of three between AS = 0.05 and AS = 0.8. Furthermore, as shown in Eq. 3 and Fig. 22, the shape of the SO₂ vertical profile is critical for accurate AMF calculation. In extreme scenarios, such as volcanic eruptions with plume altitudes around 6 km and SO₂ columns of 120 DU, the use of a simplified AMF may lead to an overestimation of total SO_2 by a factor of 1.5–2.

3. Reviewer 1: Details mostly relevant to future work. I am not quite convinced that the rather long Section 5.2 should be included in the manuscript in its current form. As far as I understood, the retrievals presented in this paper were performed using the highly simplified AMF as described in Section 3.5. Section 5.2 introduces a much more advanced AMF treatment which was not used in the rest of this work (unless I missed something?). While these results do offer some insights into the uncertainties of the simple AMF implementation, the entire Section 5.2 seems to be focused on the Box-AMF which is envisaged to be much more than just means

of error analysis for the simple AMF used here. Therefore, I would suggest to either remove the whole discussion of Box-AMF, leaving it for future publications, or introduce it properly as one of the main methods, rather than just means of error analysis as the current manuscript structure seems to suggest.

Authors: Thank you for this comment.

We have moved the Box-AMF introduction from Section 5.2 to Section 3.5, introducing it properly as one of the main methods. Section 5.2 now only keeps the application to uncertainty estimates.

The Air Mass Factor (AMF) is a crucial component in SO₂ retrievals. In this study, due to the unavailability of accurate global SO₂ vertical profile data, we applied a simplified AMF strategy (AMF=1 for clean regions and non-ice/snow-covered areas, while the other is AMF=2 for the ice/snow-covered areas). While we understand the reviewer's concern regarding Section 5.2, removing the discussion of AMF errors entirely would leave readers without guidance on the OMS SO₂ AMF uncertainties and force them to consult external literature.

In the revised manuscript (P35, L593–L603 and Figure 22), to more clearly demonstrate the biases introduced by the simplified AMF strategy, we conducted AMF calculations using SCIATRAN Box-AMFs and assumed SO₂ profiles under a range of atmospheric and surface conditions. Specifically, six SO₂ profiles were constructed, representing clean conditions, low, medium, and high anthropogenic SO₂ emissions, volcanic degassing with plume heights around 2 km, and volcanic eruptions with plume heights around 6 km.

In the revised manuscript, additional text (shown in red font below) and the corresponding figure (Fig. 22 in the revised manuscript) have been added to further elaborate on these results. As shown in the Figure 22 below, we can see that the magnitude of biases introduced by the simplified AMF approach varies significantly under different conditions.

Neglecting forward model errors, Figure 22 shows the dependence of AMF on SZA,

VZA, AS, wavelength, O₃ column, and SO₂ profiles. The AMFs were calculated with SCIATRAN Box-AMFs using six assumed SO₂ profiles. Here six SO₂ profiles were constructed, representing clean conditions, low, medium, and high anthropogenic SO₂ emissions, volcanic degassing with plume heights around 2 km, and volcanic eruptions with plume heights around 6 km. As shown in Fig. 22, although AMF values are generally close to 1 under typical atmospheric and surface conditions (non-ice/snow-covered), the magnitude of biases introduced by the simplified AMF approach (AMF=1 for clean regions and non-ice/snowcovered areas, while the other is AMF=2 for the ice/snow-covered areas) varies significantly with different conditions. Surface albedo is the major factor affecting AMF accuracy. For instance, AMFs can differ by up to a factor of three between AS = 0.05 and AS = 0.8. Furthermore, as shown in Eq. 3 and Fig. 22, the shape of the SO₂ vertical profile is critical for accurate AMF calculation. In extreme scenarios, such as volcanic eruptions with plume altitudes around 6 km and SO₂ columns of 120 DU, the use of a simplified AMF may lead to an overestimation of total SO₂ by a factor of 1.5–2. Since the actual vertical distribution of atmospheric SO₂ is often difficult to get, a priori profiles from models are commonly used in AMF calculations. For regions with anthropogenic emissions, atmospheric chemistry models like GEOS-Chem and TM5 are often used to provide global SO₂ profiles for AMF calculation. The uncertainties in these profiles can also propagate into AMF calculations. In future work, we aim to incorporate high-resolution and satellite-synchronized SO₂ vertical profiles to improve the accuracy of AMF.

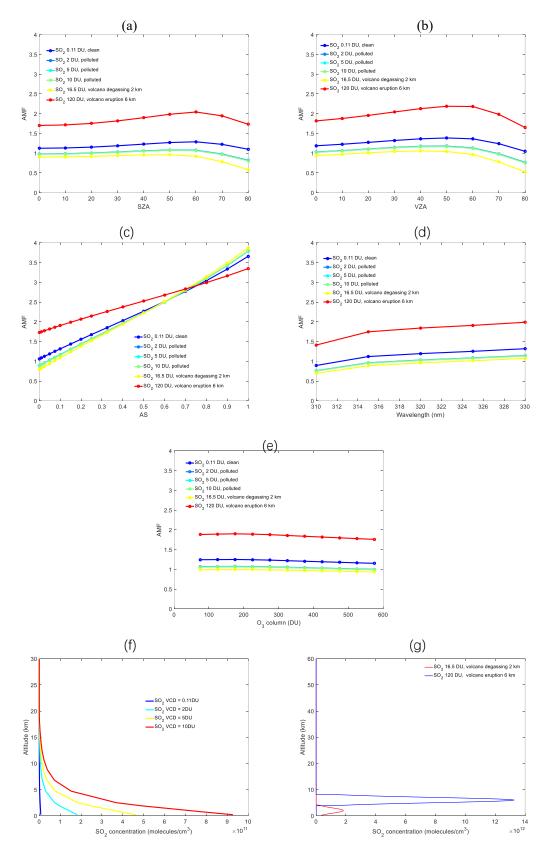


Figure 1: Dependence of AMF on SZA (a), VZA (b), AS (c), Wavelength (d), O₃ column (e), and SO₂ profiles. AMFs are calculated with SCIATRAN Box-AMFs using assumed SO₂ profiles. (f) Assumed SO₂ profiles corresponding to clean conditions, low, medium, and high anthropogenic SO₂ emissions; (g) Assumed SO₂

profiles corresponding to volcanic degassing with plume heights around 2 km, and volcanic eruption with plume heights around 6 km. The default SCIATRAN settings for Box-AMF calculation are as follows: wavelength=320 nm, clear sky, HS=0 km, O₃=275 DU, AS=0.05, SZA=32.9°, VZA=0°, RAA=0°.

4. Reviewer 1: Amount of figures. The manuscript contains a number of multipanel figures that result from repeating the same analysis on different areas (or different spectral windows, etc.). This results in a large number of multipanel figures, not all of which are adequately discussed in the main text (e.g. specific comment #1). I would suggest to remove some of the figures (or panels in the figures)

Authors: Thanks for this comment. The intention of the authors was to demonstrate the reliability of the OMS SO₂ results across different times and locations, as we were concerned that a limited number of temporal or spatial cases might not fully reflect the reliability of the OMS SO₂ retrievals. We therefore prefer to keep the figures in the manuscript.

5. Reviewer 1: Some figures do not conform to journal standards. Some figures span multiple pages and have no labels for panels. As far as I know, this does not conform to journal standards.

Authors: Thank the reviewer for pointing out this issue. In the revised manuscript, we have adjusted the figure layout to ensure, as much as possible, that each figure is presented on a single page rather than spanning multiple pages, although this could not be achieved for all figures. In addition, we have added panel labels to the relevant figures (e.g., Figure 21). Given the large number of figures, all corresponding modifications can be found in the revised manuscript. Any remaining nonconformities with journal standards will be discussed with Copernicus before publication.

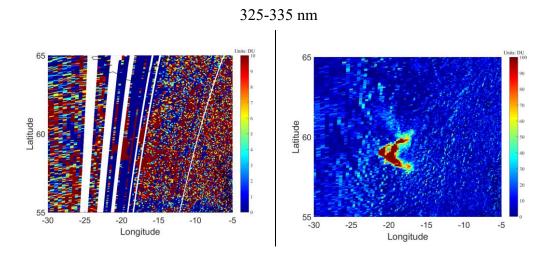
6. Reviewer 1: Figure 2: Retrievals from the spectral windows of 325–335 nm and 360–390 nm appear to be complete failures. The authors should comment on why

they failed, which would be far more useful than explicitly showing clearly unphysical retrieval results in (already overloaded) figures 2 and 3. The statement that a lot of NaN values were produced by the retrieval is very uninformative in this case.

Authors: Thank you for this comment and suggestion.

In the previous version of the manuscript, the SO₂ retrievals in these windows showed a large number of missing data. This was because the minimum value in the retrieval code had been set to –100 DU, and values lower than this were treated as outliers and assigned as Nan. After background offset correction, this led to a large number of missing values in the 325–335 nm and 360–390 nm retrievals over the Sundhnúkur volcano on August 23, 2024. In the revised manuscript, considering the broader variability of retrievals in the 325–335 nm and 360–390 nm windows, we reset the minimum value to –4000 DU. As a result, the missing data problem in Figure 2 has been largely eliminated. It should be noted that in the revised manuscript, we have also updated the 325–335 nm and 360–390 nm retrievals in Figure 2 (P8) by applying a different color scale range (0–100 DU and 0-400 DU) in order to better present the retrieval results (as shown in the figures below). In addition, we have updated the 325–335 nm and 360–390 nm retrievals in Figure 3 (P9) correspondingly.

We would like to emphasize that not only the SO₂ retrievals from the 325–335 nm and 360–390 nm windows in volcanic regions are generally higher than those from the 312–326 nm window, but also their standard deviations are quite large, even over clean and homogeneous oceanic regions.



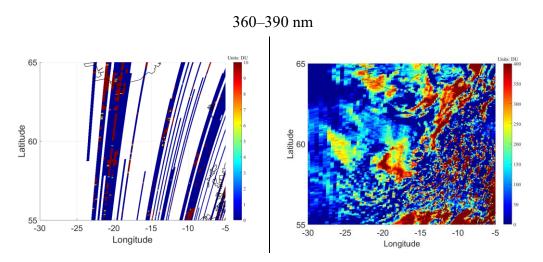


Figure: SO_2 retrievals from 325–335 nm and 360–390 nm fitting windows over the Sundhnúkur volcano on August 23, 2024 (OMS orbit 20240823_1036). DU=Dobson Units, 1 DU= 2.69×10^{16} molecules/cm². The left panel shows the figures from the previous version of the manuscript, while the right panel shows the updated figures from the revised manuscript.

7. Reviewer 1: L114: "ISRF exhibits a flat top". Ideally, this should be accompanied by a figure or reference, so that the reader can get a sense of the nature and extent of the problem.

Authors: Thank you for this comment. In the paper "Preflight Spectral Calibration of the Ozone Monitoring Suite-Nadir on FengYun-3F Satellite" by

Wang Qian (2024), relevant figures and descriptions illustrating the issue of "ISRF exhibits a flat top" are provided. A screenshot of the figure from Wang's paper is shown below for reference. We have also added the corresponding citation in the revised manuscript.

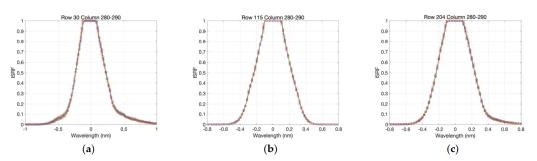


Figure 9. Samples from 11 spectral pixels in the VIS band are combined to give a single set of data, with a higher resolution shown by the colored circles. (a) Row 30; (b) row 119; (c) row 204.

8. Reviewer 1: L83-95: This paragraph contains a list of eight points. I think using numbers and/or special formatting would be more helpful to the reader than words like "seventhly".

Authors: We agree with this suggestion. In the revised manuscript (L84-97), we have added numbering (e.g., (1), (2), ...) to the eight points to make the paragraph clearer and more reader-friendly.

9. Reviewer 1: L133: Present tense here would be more consistent with the rest of the paragraph.

Authors: This has been corrected in the revised manuscript (L134).

10. Reviewer 1: Figure 4 caption: I would suggest not to provide so many numerical values in a caption, but rather present them in a table, either as part of Figure 4 or separately.

Authors: We agree with this suggestion. In the revised manuscript, we have presented the standard deviations and means of the different fitting windows as part of Figure 4, and removed the numerical descriptions from the caption. A screenshot

of the revised Figure 4 is attached here.

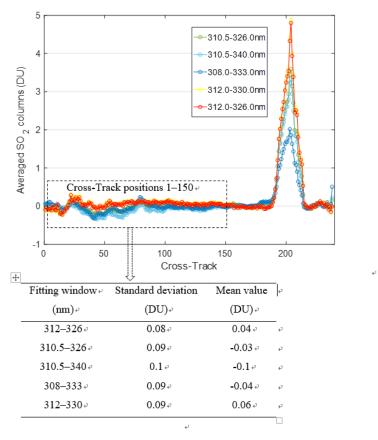


Figure 4: Row-averaged SO₂ retrievals from OMS rows 700 to 870 of orbit 20240823_1036 by using different spectral fitting windows.

11. Reviewer 1: L343: The comparison of results from [...].

Authors: This has been corrected in the revised manuscript.

12. Reviewer 1: L503: Replace "difficult to be monitored and calibrated" with "difficult to monitor and calibrate".

Authors: Thank the reviewer for pointing out this language issue. We have revised the sentence in the revised manuscript (L496), replacing "difficult to be monitored and calibrated" with "difficult to monitor and calibrate".