Title: Retrieval of SO_2 columns from FY3F/OMS instrument observations

Authors: Huanhuan Yan, Andreas Richter, Xingying Zhang, Anja Schönhardt, and 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 #2

1. **Reviewer 2:** The authors refer to this as the "first version" of the OMS SO_2. It would be useful to clearly state this in the title or abstract to manage reader expectations about its development stage and limitations.

   Authors: Thanks for this recommendation. We agree with this comment. The title of the manuscript has been revised to "First results of SO_2 columns from FY3F/OMS instrument observations" to reflect the limitations of the current version and to indicate the early stage of its development. In addition, at the end of the abstract, we have included the sentence "This study is the first to present SO_2 retrievals from FY3F/OMS observations" to further clarify this point.

2. **Reviewer 2:** The paper (L95-96) recommends filtering OMS data for SZA < 70 °, near-nadir, and cloud-free pixels. Were these recommended filters (including cloud-free) applied to the OMS data before comparison with TROPOMI? Please clarify the exact filtering used, especially given the statement about no cloud products.

Authors: We are sorry for the unclear statement. When comparing with TROPOMI, we filtered OMS SO_2 retrievals greater than –10 DU, but did not apply filtering for pixels with cloud coverage or large SZA. In other words, OMS SO_2 retrievals with cloud coverage or large SZA were included in the comparison with TROPOMI SO_2 results as long as they were greater than –10 DU. To clarify this point, we have added the following description at the end of the first paragraph in Section 4 (L290-292) of the revised manuscript (in red font):

"It should be noted that, in the comparison between OMS and TROPOMI SO_2 results, no filtering for cloud or SZA was applied to the OMS SO_2 data; instead, all retrievals greater than –10 DU were selected for the comparison."

3. **Reviewer 2:** The paper mentions the use of the TSIS HSRS hybrid solar reference spectrum instead of OMS L1 solar irradiance due to degradation. Could this lead to systematic biases in the long term? What plans are in place to account for this degradation?

Authors: For FY-3F/OMS SO_2 retrievals, it is essential to obtain accurate solar irradiance data for calculating the TOA reflectance (radiance/irradiance). However, after one year in orbit, we found that the intensity of OMS irradiance at the shorter wavelength of 317 nm had decreased by about 8.83%, while at the longer wavelength of 331 nm it had decreased by about 6.07%. This degradation in OMS solar irradiance measurements is one of the main causes of the systematic low bias and striping observed in OMS trace gases retrievals, especially for ozone products.

In addition to the solar irradiance issue, OMS radiance measurements also suffer from certain calibration errors. The combined effect of these issues has led to systematic biases in the retrievals of OMS trace gases, as well as striping and left–right asymmetry problems. Given these multiple issues, we prioritized addressing the striping and left–right asymmetry problems by using the TSIS HSRS hybrid solar reference spectrum instead of the OMS L1 solar irradiance for total SO_2 retrievals. To date, the work on correcting the calibration errors in OMS L1

radiance and irradiance is still ongoing.

Using the TSIS HSRS hybrid solar reference spectrum can mitigate the effects of viewing-angle dependence and degradation on OMS SO_2 retrievals. However, because the solar reference spectrum does not include the instrument's specific characteristics, it may introduce systematic overestimation or underestimation in SO_2 column retrievals, and these errors could change over time. Such systematic biases introduced by the TSIS HSRS can be partially reduced through background offset correction, but they cannot be completely eliminated.

For the retrieval of atmospheric composition from OMS, using the OMS measured irradiance data can reduce some errors, and our preliminary plan for correcting the degradation of OMS irradiance in the future is to first correct the degradation in the ultraviolet region, and then analyze the changes in the OMS diffuser based on the existing OMS irradiance observations for subsequent improvements.

4. **Reviewer 2:** The results in Figure 2 from using the 325–335 nm and 360–390 nm windows alone appear unconvincing. While these windows might be noisy in isolation, their value (as seen in TROPOMI's algorithm) lies in their combined use with stronger windows to avoid saturation at high SO_2 Since OMS shows saturation and underestimation for high SO_2, have the authors explored a multi-window fitting strategy to improve this?

Authors: Thank you for this comment and suggestion. In general, it is well known that in volcanic eruption cases with high SO_2 columns, retrievals using strong SO_2 absorption bands are often subject to saturation effects. By contrast, retrievals using weaker SO_2 absorption bands in the longer UV range can effectively mitigate this saturation. The reviewer's suggestion is therefore very good and is indeed in line with our future plan for the OMS SO_2 product.

Our preliminary strategy for future OMS SO_2 retrievals during volcanic eruptions is as follows. (1) Initial retrieval: Use the 312–326 nm window to perform a global SO_2 column retrieval. (2) Flagging potential saturation: Pixels with SO_2 columns

above a certain threshold (e.g., >50 DU) are flagged as potentially affected by saturation at high SO_2. For these flagged pixels, additional retrievals are conducted using the 325–335 nm and 360–390 nm windows. (3) Assessment and replacement: The SO_2 values from the 325–335 nm and 360–390 nm windows are assessed to determine whether they fall within a reasonable range and exceed the corresponding 312–326 nm values. If both conditions are satisfied, the 312–326 nm retrievals are replaced by the maximum of the 325–335 nm or 360–390 nm values; otherwise, the original 312–326 nm retrievals are retained. In the revised manuscript, an abbreviated version of this plan has been added to Section 6 (L686-691), as indicated in red font below.

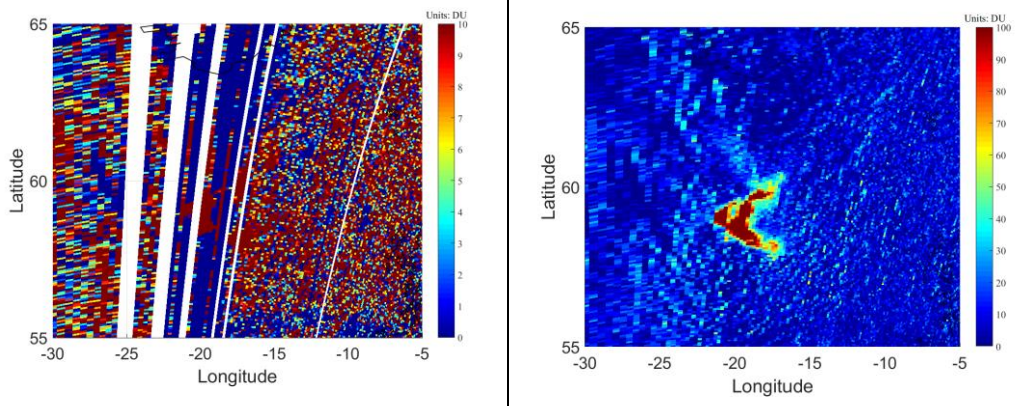
Our preliminary strategy for such retrievals is as follows. First, a global SO_2 column retrieval is performed using the 312–326 nm window. Pixels exceeding a threshold (e.g., >50 DU) are flagged as potentially saturated. For these flagged pixels, additional retrievals are conducted using the 325–335 nm and 360–390 nm windows. If the new retrievals are within a reasonable range and exceed the 312–326 nm results, the maximum value from the 325–335 nm or 360–390 nm windows replaces the original retrieval; otherwise, the 312–326 nm retrieval is retained.

In addition, 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 figure below). In the previous version of the manuscript, the SO_2 retrievals in these windows showed a large amount 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 this 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. In addition, we have correspondingly updated the 325–335 nm and 360–390 nm retrievals in Figure 3 (P9).

We would like to emphasize that not only the SO_2 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.

325-335 nm



360–390 nm

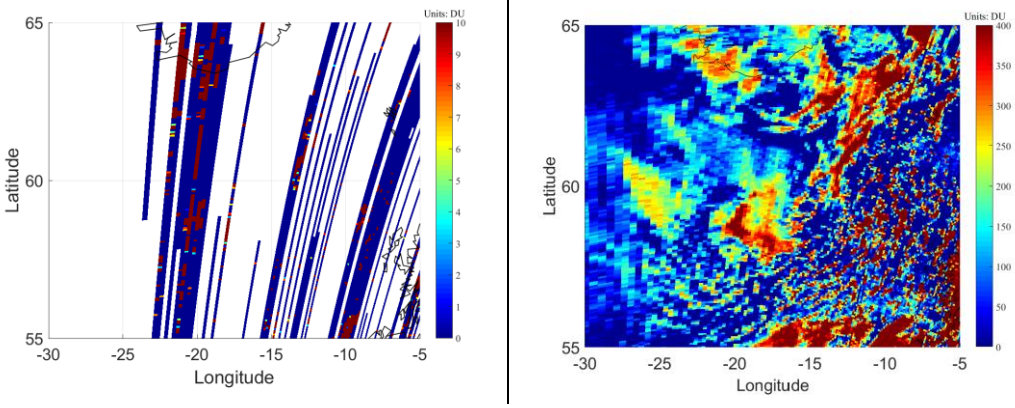


Figure: SO_2 retrievals from 325–335 nm and 360–390 nm fitting windows over the Sundhnúkur volcano on August 23, 2024 (OMS orbit 20240823_1036). DU=Dobson Units, 1 DU=2.69×10^{16} molecules/cm^2. The left panel shows the figure from the previous version of the manuscript, while the right panel shows the updated figure in

the revised manuscript.

5. **Reviewer 2:** Section 3.3.2 states a single fixed Ring spectrum was used. However, Figure 19 clearly shows the Ring spectrum varies significantly with atmospheric and viewing conditions. Please clarify this apparent contradiction: was a single fixed Ring spectrum or a variable one used? If a single fixed spectrum was used, the significant error introduced by ignoring these variations should be quantitatively discussed and the actual Ring spectrum settings should be reflected in Table 3.

Authors: Thanks for pointing this out, and sorry for the inaccurate description in the original manuscript. In this study, one single Ring spectrum simulated with the SCIATRAN model was used to retrieve OMS SO_2 for all pixels. As we know, the Ring effect in the UV wavelength range is a non-negligible component of the DOAS SCD fitting process. Initially, we generated a lookup table for the 310–330 nm wavelength range using the SCIATRAN model, considering variations in SZA, VZA, O_3 column, and AS to achieve more accurate retrievals. However, this lookup table is large and significantly increased computational cost for OMS SO_2 retrievals. Moreover, the OMS SO_2 retrievals indicate that the impact of the Ring spectrum variability on SO_2 retrievals is relatively small for high SO_2 concentrations, due to the weak correlation between the Ring spectrum and the satellite TOA reflectance. Therefore, in this study, we adopted the approach of using a single Ring spectrum for all OMS pixels.

To clarify this point, in the revised manuscript, the original text in Section 5.1 (blue font) has been modified and replaced with the following text (red font).

In the UV wavelength band, the Ring effect is a non-negligible part of the DOAS SCD fitting process. In this study, one single Ring spectrum simulated with the SCIATRAN model was used to retrieve OMS SO_2 for all pixels. As shown in Fig. 19, the Ring spectrum convolved with the OMS ISRF varies with SZA, VZA, O_3 column and AS within the 310–330 nm wavelength range. The variation of the

Ring spectrum with RAA is negligible and is not presented in this study. The mean percentage change in the Ring spectrum is approximately 27.67% (absolute deviation: 0.0025) as the O_3 column varies from 175 DU to 575 DU, 47.34% (absolute deviation: 0.0048) as the AS varies from 0 to 1, 24.18% (absolute deviation: 0.0021) as the VZA varies from 0° to 75°, and 45.29% (absolute deviation: 0.0047) as the SZA varies from 0° to 80°. Although the Ring spectrum varies significantly with SZA, VZA, O_3 column, and AS within the 310–330 nm wavelength range, its impact on SO_2 retrievals is relatively small for high SO_2 concentrations due to the weak correlation between the Ring spectrum and the satellite TOA reflectance. However, for low SO_2 concentrations, the influence is non-negligible.

In the UV wavelength band, the Ring effect is a non-negligible part of the DOAS SCD fitting process. As shown in Fig. 19, the Ring spectrum convolved with the OMS ISRF varies with SZA, VZA, O_3 column and AS within the 310–330 nm wavelength range. The variation of the Ring spectrum with RAA is negligible and is therefore not presented. The mean percentage change in the Ring spectrum is approximately 27.67% (absolute deviation: 0.0025) as the O_3 column varies from 175 DU to 575 DU, 47.34% (absolute deviation: 0.0048) as the AS varies from 0 to 1, 24.18% (absolute deviation: 0.0021) as the VZA varies from 0° to 75°, and 45.29% (absolute deviation: 0.0047) as the SZA varies from 0° to 80°. However, in this study, a single Ring spectrum simulated with the SCIATRAN model was used to retrieve OMS SO_2 for all pixels. The reason is that although the Ring spectrum varies significantly with SZA, VZA, O_3 column, and AS within the 310–330 nm wavelength range, the impact of Ring spectrum variability on SO_2 retrievals is relatively small due to the weak correlation between the Ring spectrum and the satellite TOA reflectance, especially in the case of volcanic eruptions with high SO_2 concentrations. Moreover, using Ring spectra that vary with SZA, VZA, O_3 column, and AS within the 310–330 nm wavelength range require constructing a large lookup table, which would significantly increase computational cost for

OMS SO_2 column retrievals.

6. **Reviewer 2:** What improvements are considered at orbit edges in a future update?

   Authors: At orbit edges, the retrieval accuracy is relatively low due to large viewing angles. This issue is also present in other satellite instruments such as TROPOMI and GOME-2. Ongoing improvements to the OMS L1 data are being made to reduce striping and asymmetry in the calibration to improve SO_2 retrieval accuracy. Despite several attempted corrections, no effective strategy for the edge pixels is currently available and therefore we recommend that users take caution when using them. Nevertheless, the different overpass time and spatial coverage of OMS compared to other satellite instruments allow OMS to provide complementary observations, particularly for TROPOMI orbit edge pixels and in the tropical orbit gap regions.

7. **Reviewer 2:** For the Persian Gulf, the 0.5-0.6 correlations are not particularly high. What does this imply regarding the agreement between the OMS and TROPOMI products, and what factors contribute to these differences?

   Authors: We agree that in the Persian Gulf region, the correlation coefficient of 0.5–0.6 is not high. We consider that this may be related to the following factors: (1) the different overpass times of OMS (morning, about 10:00 am) and TROPOMI (afternoon, about 13:30 pm), during which atmospheric conditions may have changed, leading to discrepancies; (2) the differences in viewing geometries between the two instruments; (3) Random noise and uncertainties from background correction, which are relevant for low SO2 scenarios, such as over the Persian Gulf, in data from both instruments and lead to scatter in the order of several DU.

   In addition, the differences among the three datasets (OMS SO_2, TROPOMI DOAS SO_2, and TROPOMI COBRA PBL SO_2) vary over time: on August 23, 2024, OMS SO_2 retrievals were higher than those from both TROPOMI DOAS and TROPOMI COBRA, whereas on November 12, 2024, OMS SO_2 retrievals were lower than

those of TROPOMI DOAS and TROPOMI COBRA.

8. **Reviewer 2:** How much does the difference of the overpass time between OMS and TROPOMI contribute to the observed differences in SO_2 retrievals, particularly in dynamic regions like volcanic or strong anthropogenic plumes?

   Authors: Thanks for this comment. The difference in overpass time between OMS and TROPOMI can contribute to the observed discrepancies in SO_2 retrievals, particularly in regions with rapidly changing SO_2 concentrations, such as those affected by volcanic or strong anthropogenic plumes. However, isolating and quantifying the sole impact of overpass time requires accurate knowledge of the temporal evolution of SO_2 emissions and meteorological conditions within the time window between the OMS and TROPOMI overpasses, which is challenging for the current study. Our focus here is therefore on the overall differences between OMS and TROPOMI.

   Nevertheless, in high-latitude regions, OMS and TROPOMI often provide multiple orbital coverages of the same area within a short period, which offers opportunities to see their SO_2 retrieval differences under relatively small overpass time differences. For example, as shown in Fig. 12, the Sundhnúkur volcano in the Northern Hemisphere high latitudes was captured by multiple OMS orbits, enabling near-simultaneous comparisons with TROPOMI. Compared with OMS orbit 20240823_1036, OMS orbit 20240823_1217 has a local overpass time closer to that of the TROPOMI orbit 20240823T125304 in the volcanic region, resulting in more consistent SO_2 retrievals between OMS and TROPOMI.

   Future work employing high-temporal-resolution satellite observations (e.g., GEMS, TEMPO) or chemical transport model simulations could provide more detailed insights into the role of overpass time differences.

9. **Reviewer 2:** The paper highlights the simplified AMF approach as introducing significant errors and large uncertainties. Could the authors elaborate further on the

estimated magnitude of biases introduced by these simplifications across a range of atmospheric and surface conditions? Furthermore, to enhance the accuracy and robustness of the product, particularly in complex regions like urban areas or near industrial sources, what are the plans for incorporating a more physically-based AMF calculation?

Authors: Thank you for this comment. Our responses are as follows:

1) **Comment:** The paper highlights the simplified AMF approach as introducing significant errors and large uncertainties. Could the authors elaborate further on the estimated magnitude of biases introduced by these simplifications across a range of atmospheric and surface conditions?

   Answer: Thanks for this revision suggestion. We agree with the reviewer that using a simplified AMF (AMF=1 for clean regions and non-ice/snow-covered areas, while the other is AMF=2 for the ice/snow-covered areas) to convert slant columns to vertical columns introduces errors, particularly under complex atmospheric and surface conditions. The AMF value is influenced by multiple factors, including wavelength, solar zenith angle (SZA), viewing zenith angle (VZA), relative azimuth angle (RAA), surface albedo (AS), terrain height (HS), O_3 column, SO_2 vertical profile shape, and cloud fraction and altitude.

   In the revised manuscript, we conducted AMF calculation by using SCIATRAN Box-AMFs and SO_2 profiles under a range of atmospheric and surface conditions to analyze the biases between simplified AMF and physically-based AMF. Specifically, we constructed six SO_2 profiles corresponding to clean conditions, low, medium, and high anthropogenic SO_2 emissions, volcanic degassing with plume heights around 2 km, and volcanic eruption with plume heights around 6 km.

   Neglecting forward model errors, the figure below shows that the magnitude

of biases introduced by the simplified AMF approach varies significantly under different conditions. In the revised manuscript, additional text (L593-603, shown in red font below) and the corresponding figure (Fig. 22 in the revised manuscript) have been added to further elaborate on these results.

Neglecting forward model errors, Figure 22 shows the dependence of AMF on SZA, VZA, AS, wavelength, HS, O_3 column, and SO_2 profiles. The AMFs were calculated with SCIATRAN Box-AMFs using assumed SO_2 profiles. 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/snow-covered 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 SO_2 vertical profile is critical for accurate AMF calculation. In extreme scenarios, such as volcanic eruptions with plume altitudes around 6 km and SO_2 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. Since the actual vertical distribution of atmospheric SO_2 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 SO_2 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 SO_2 vertical profiles to improve the accuracy of AMF.

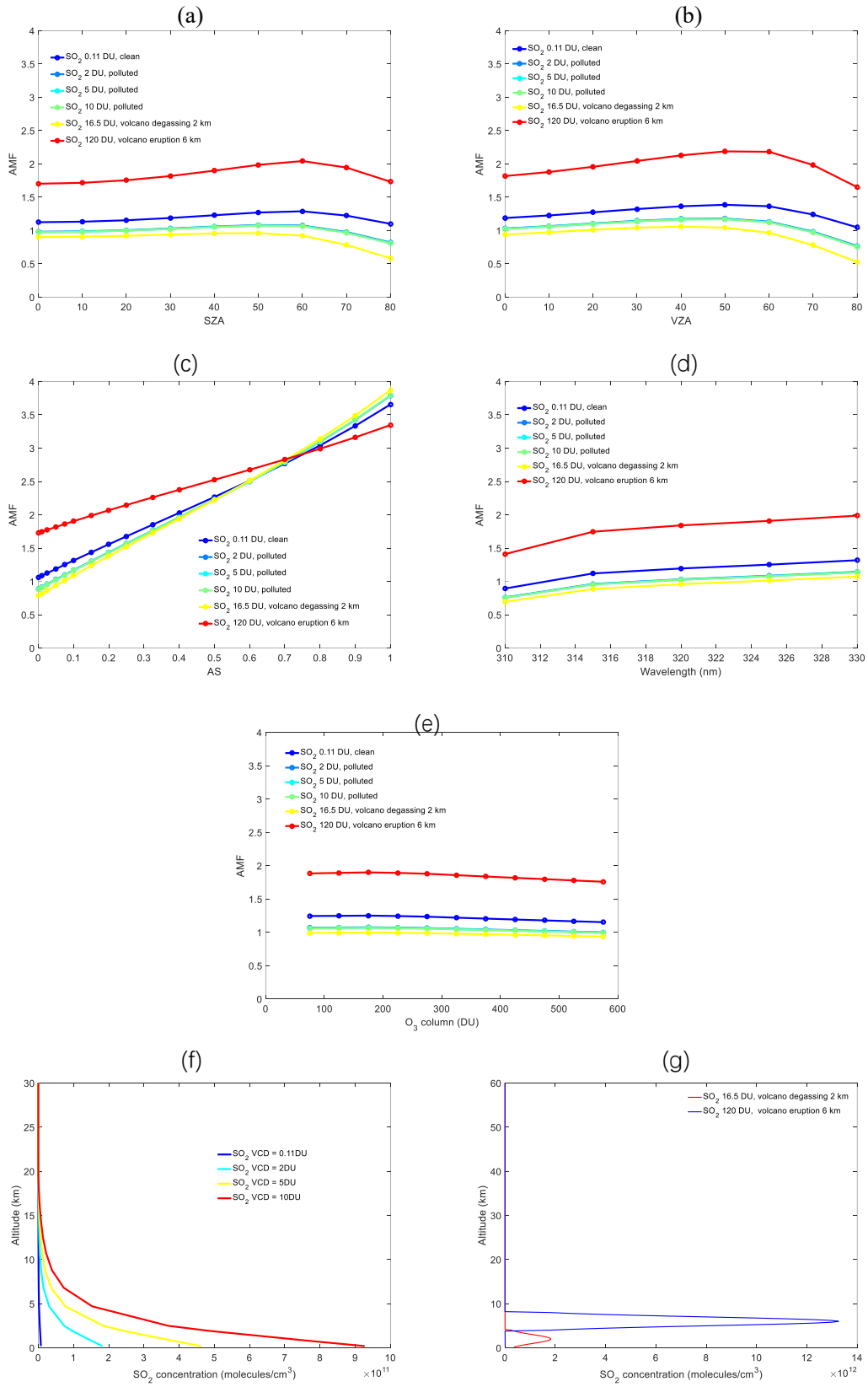


Figure 1: Dependence of AMF on SZA (a), VZA (b), AS (c), Wavelength (d), O_3 column (e), and SO_2 profiles. AMFs are calculated with SCIATRAN Box-AMFs using assumed SO_2 profiles. (f) Assumed SO_2 profiles corresponding to

clean conditions, low, medium, and high anthropogenic SO_2 emissions; (g) Assumed SO_2 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, O_3=275 DU, AS=0.05, SZA=32.9°, VZA=0°, RAA=0°.

2) **Comment:** Furthermore, to enhance the accuracy and robustness of the product, particularly in complex regions like urban areas or near industrial sources, what are the plans for incorporating a more physically-based AMF calculation?

Answer: We thank the reviewer for their comment on the importance of a more physically-based AMF calculation, especially for improving retrievals in complex regions such as urban or industrial areas. Until now, we have been exploring collaboration with other research teams to obtain more accurate SO_2 vertical profiles representative of regions with anthropogenic emissions.

In future work, once high-resolution and accurate SO_2 profiles become available, we plan to develop an offline product. This offline product will employ more accurate AMFs to reprocess historical data and thereby improve the accuracy of the retrievals, particularly in regions with strong or anthropogenic emissions.

10. Reviewer 2: The current retrieval does not account for cloud and aerosol effects, which can introduce significant biases, particularly for boundary layer SO_2. What are the plans to integrate cloud and aerosol effects into future updates of the retrieval algorithm?

Authors: Thanks for this valuable comment. We agree that neglecting cloud and aerosol effects may introduce significant biases, especially for boundary layer SO_2 retrievals. Our plans for future updates are as follows:

(1) Short-term strategy: In the absence of reliable OMS cloud and aerosol products, we recommend users to primarily use clear-sky pixels. A simple radiance-based screening will be implemented to flag cloud-contaminated pixels in the SO_2 output file. In addition, cloud products from other instruments (e.g., TROPOMI, OMI, MODIS, or MERSI) may be incorporated as auxiliary inputs to reduce cloud-related uncertainties.

(2) Long-term strategy: Once mature OMS cloud and aerosol products become available, they will be integrated into the retrieval algorithm to enable accurate AMF calculations. This will significantly improve the accuracy of SO_2 retrievals, particularly for the boundary layer. Furthermore, quality control flags will be refined (e.g., pixels with cloud fraction > 0.3 or strong aerosol events will be filtered or flagged as low quality) to facilitate more reliable usage of the OMS SO_2 product.