

# First results of SO<sub>2</sub> columns from FY-3F/OMS instrument observations

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**Abstract.** Atmospheric SO<sub>2</sub> has a significant impact on the urban environment and on global climate. Remote sensing provides an unprecedented tool for the continuous and real-time monitoring of atmospheric SO<sub>2</sub> from volcanic eruptions and anthropogenic emissions. The Ozone Monitoring Suite (OMS) onboard the Chinese FENGYUN-3F (FY-3F) satellite launched in August 2023 is a new hyperspectral UV-VIS instrument in the FY-3 family of satellites, aiming to obtain information about atmospheric trace gases. In this study, we use the OMS Nadir (OMS-N) top-of-atmosphere (TOA) measurements and Differential Optical Absorption Spectroscopy (DOAS) inversion to for the first time retrieve global SO<sub>2</sub> columns from these measurements. 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 found in the raw OMS SO<sub>2</sub> retrievals. The accuracy of FY-3F/OMS SO<sub>2</sub> retrievals was evaluated by comparing them with the DOAS and COvariance-Based Retrieval Algorithm (COBRA) SO<sub>2</sub> products from the TROPOspheric Monitoring Instrument (TROPOMI) onboard Copernicus Sentinel-5 Precursor (Sentinel-5P) over three typical areas: clean oceanic regions, volcanic eruption regions, and anthropogenic emission regions. The results indicate that the OMS SO<sub>2</sub> retrievals exhibit good stability over clean oceanic regions (with a precision of approximately 0.15 DU), successfully capture volcanic SO<sub>2</sub> plumes, and effectively detect the elevated SO<sub>2</sub> columns from anthropogenic emissions in regions such as the Middle East, Eastern India, and Northern Russia. Detector non-uniformity and Air mass factor (AMF) uncertainty remains the primary error source of this first version of OMS SO<sub>2</sub> retrievals. This study is the first to present SO<sub>2</sub> retrievals from FY-3F/OMS observations, which is crucial for a comprehensive understanding of OMS's capability in SO<sub>2</sub> retrievals.

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## 1 Introduction

Sulfur dioxide (SO<sub>2</sub>) is a short-lived trace gas in the atmosphere that affects regional air quality and global climate change. SO<sub>2</sub> is primarily released by anthropogenic activities (e.g., smelting of sulfur ore, combustion of coal, the oil and gas industry, emissions of motor vehicles) and natural phenomena (e.g., volcanic and biological processes) (Finlayson-Pitts and Pitts Jr, 1999; Cullis and Hirschler, 1980; Seinfeld and Pandis, 2016). SO<sub>2</sub> injection from a volcanic eruption can reach up to the upper troposphere/lower stratosphere, not only affecting global climate but also posing a threat to aviation, along with volcanic ash. Through reaction with hydroxyl radicals (OH) and water, atmospheric SO<sub>2</sub> can be rapidly converted into sulfate aerosols. These aerosols both scatter and absorb solar and terrestrial radiation, affecting the radiation balance of the atmosphere (cooling or warming effect) (Twomey, 1977). Sulfate particles formed from anthropogenic SO<sub>2</sub> emissions not only influence atmospheric visibility in the boundary layer but also contribute to acid rain which in turn damages ecosystems.

Low-Earth-orbit (LEO) satellite remote sensing offers the advantages of near global coverage, short-term periodic observation capabilities, and continuous spatial coverage. Due to the strong absorption characteristics of SO<sub>2</sub> in the ultraviolet (UV) spectrum, especially in the 300–400 nm wavelength range, atmospheric SO<sub>2</sub> information can be obtained from the reflected TOA radiance spectrum. Since the first UV-based satellite observation of large amounts of SO<sub>2</sub> from the El Chichón volcanic eruption in 1982 by TOMS (Krueger, 1983), hyperspectral UV satellite instruments have been used to quantitatively monitor the spatial and temporal distribution of SO<sub>2</sub> and its dispersion following volcanic eruptions. This compensates for the limitations of ground-based measurements, such as the high cost of dense in-situ observation networks and instrument maintenance (Krueger, 1983; Carn et al., 2005; Carn et al., 2007; Carn et al., 2009).

With the launch of a series of hyperspectral UV detection instruments, including the Global Ozone Monitoring Experiment (GOME) (Burrows et al., 1999; Khokhar et al., 2005; Eisinger and Burrows, 1998), the Scanning Imaging Absorption Spectrometer for Atmospheric Cartography (SCIAMACHY) (Gottwald and Bovensmann, 2010; Richter et al., 2006), the Ozone Monitoring Instrument (OMI) (Levelt et al., 2006), the Global Ozone Monitoring Experiment-2 (GOME-2) (Heue et al., 2010; Munro et al., 2006; Richter, 2009), the Ozone Mapping and Profiler Suite (OMPS) (Yang et al., 2013; Flynn et al., 2006), TROPOMI (Theys et al., 2019; Voors et al., 2017; Veeffkind et al., 2012), and the Environmental Trace Gas Monitoring Instrument (EMI) (Chen et al., 2021; Zhao et al., 2020; Yan et al., 2021), satellite detection has been widely applied to monitor global SO<sub>2</sub> variations and to support research on climate change, atmospheric chemistry, and the atmospheric environment.

FY-3F/OMS is a newly launched Chinese UV-VIS hyperspectral sensor that provides global observations with 7 km × 7 km spatial resolution at nadir and a morning overpass time. For a thorough understanding of the OMS SO<sub>2</sub> product, this study presents OMS SO<sub>2</sub> retrievals by using the OMS measurements and DOAS inversion, and compares them with TROPOMI DOAS and TROPOMI COBRA SO<sub>2</sub> products over clean oceanic regions, volcanic eruption regions, and anthropogenic emission regions. This paper is organized as follows. Section 2 gives a brief introduction to the FY-3F/OMS instrument. Section 3 describes the detailed procedures used to retrieve the SO<sub>2</sub> columns from FY-3F/OMS observations, including solar

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80 spectrum selection, spectral soft calibration, SO<sub>2</sub> slant column density (SCD) retrieval, background offset correction, and the  
 approach for AMF calculation used. Section 4 provides the OMS SO<sub>2</sub> column results, followed by comparisons with the  
 TROPOMI DOAS and TROPOMI COBRA SO<sub>2</sub> products. Section 5 discusses error sources of OMS SO<sub>2</sub> retrievals,  
 including the instrument-related errors and DOAS SCD spectral fitting errors in OMS SO<sub>2</sub> SCD retrievals, errors introduced  
 by the AMF approach taken, and the residual errors after background offset correction. The last section summarizes the main  
 85 results and offers conclusions, along with suggestions for future improvements.

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## 2 The FY-3F/OMS Instrument

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**Table 1. The main characteristics of the FY-3F/OMS-N instrument**

Parameter	Nadir column measurement	Nadir profile measurement
Spectral range	VIS: 307~493nm	UV1:250~300nm UV2: 300~320nm
Spectral resolution	0.5~0.6nm	UV1: ~1.0nm UV2: ~0.5nm
Spectral accuracy	0.01nm	0.05nm
Spatial resolution at nadir point	7 km x 7 km	UV1: 21 km x 28 km UV2: 7 km x 7 km
Atmospheric products	O <sub>3</sub> , NO <sub>2</sub> , SO <sub>2</sub> , HCHO, AOD, cloud fraction and pressure	O <sub>3</sub> profile
Field of view	112°	
Orbit observation	polar sun synchronous morning orbit	
Orbit altitude	836 km	
Equator crossing time	10:00 AM ( <a href="#">local time</a> )	
Duty Cycle	Daytime only	
Revisit Time:	24 hours	

90 The FY-3F satellite, the 21st in China's FengYun series, was successfully launched on August 3, 2023. It operates in a sun-  
 synchronous orbit at an altitude of 836 km, with a descending node equatorial overpass time of 10:00 AM. Equipped with 10  
 advanced atmospheric instruments, FY-3F is designed to provide high-quality data for weather forecasting, climate  
 monitoring, and environmental research, contributing significantly to global meteorological and environmental observations.  
 The Ozone Monitoring Suite (OMS) onboard FY-3F satellite is a new instrument in the FY-3 family of satellites. It has two  
 observation modes: Nadir (OMS-N) and Limb (OMS-L) (Wang et al., 2024). While OMS-L provides information on the  
 95 vertical distribution of O<sub>3</sub>, OMS-N is mainly used to obtain column information on trace gases such as O<sub>3</sub>, NO<sub>2</sub>, SO<sub>2</sub>, and

HCHO, and aerosols, as well as vertical profiles of O<sub>3</sub>. OMS-N operates using a push-broom observation technique to obtain daily global measurements, with a wide Field of View (FOV) of 112°. It incorporates two imaging grating spectrometers covering the UV (250-320 nm) and VIS (307-493 nm) bands, where the UV measurements are divided into the UV1 (250-300 nm) and UV2 (300-320 nm) sub-bands. Each spectrometer uses a 1024 × 1024 pixel imaging array, with one dimension recording spatial information along the slit and the other recording spectral information. To enhance the signal-to-noise ratio (SNR) of the original detector rows, OMS L1 applied an onboard spatial binning strategy: sets of 16 pixels were averaged to yield 58 cross-track spatial rows in the UV1 band, and 4 pixels were averaged to produce 238 cross-track spatial rows in the UV2 and VIS bands, respectively (Wang et al., 2024). The remaining spatial rows were reserved for calibration purposes. The OMS-N VIS band (307-493 nm) was used for the retrieval of OMS SO<sub>2</sub> columns in this study. It has a high spatial resolution of 7 km x 7 km at the nadir point, with a spectral resolution of 0.5-0.6 nm (Table 1). FY-3F/OMS data can be downloaded from the website <http://data.nsmc.org.cn/DataPortal/en/home/index.html>.

### 3 SO<sub>2</sub> column retrievals from FY-3F/OMS

The SO<sub>2</sub> retrieval from FY-3F/OMS involves radiance normalization, spectral soft calibration, convolution of SO<sub>2</sub> and O<sub>3</sub> cross-sections and Ring spectrum with the OMS-N Instrument Spectral Response Function (ISRF), DOAS fitting to obtain SO<sub>2</sub> SCD, AMF conversion to vertical column density (VCD), and background offset correction to reduce striping and across-track asymmetries. It should be noted that, due to the current unavailability of synchronized and reliable OMS cloud and aerosol products, the effects of clouds and aerosol on SO<sub>2</sub> retrievals were not considered in this study. For the OMS SO<sub>2</sub> product, it is recommended to use retrieval results with a solar zenith angle smaller than 70°, near-nadir and cloud-free pixels.

#### 3.1 Solar irradiance

Using the satellite measured solar irradiance for the DOAS SO<sub>2</sub> retrieval can effectively reduce instrument-related errors. However, due to the degradation and non-uniformity of the diffuser plate of OMS, the OMS L1 irradiance measurements experienced increasing errors after launch, especially in the shortwave UV region. For example, after one year on orbit, the intensity of OMS irradiance at the shorter wavelength of 317 nm has decreased by about 8.83%, while at the longer wavelength of 331 nm, it has decreased by about 6.07%. Therefore, in this study the Total and Spectral Solar Irradiance Sensor-1 (TSIS-1) Hybrid Solar Reference Spectrum (HSRS) hybrid solar reference spectrum (Coddington et al., 2021) was used for OMS SO<sub>2</sub> retrievals instead of OMS daily measured solar irradiance. The TSIS-1 HSRS hybrid solar reference spectrum was developed by normalizing high spectral resolution solar datasets to the absolute irradiance scale of the TSIS-1 Spectral Irradiance Monitor (SIM) and the CubeSat Compact SIM (CSIM). The high spectral resolution solar data are sourced from the Air Force Geophysical Laboratory (AFGL) ultraviolet solar irradiance balloon observations, the ground-based Quality Assurance of Spectral Ultraviolet Measurements in Europe Fourier Transform Spectrometer (QASUMEFTS) solar irradiance observations, the Kitt Peak National Observatory (KPNO) solar transmittance atlas, and the semi-empirical

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**Deleted:** The SO<sub>2</sub> retrieval from FY3F/OMS mainly involves the following steps. (1) Firstly, the OMS-N L1 earth radiance is normalized to the Earth-Sun distance of 1AU, while the solar irradiance is obtained by convolving the Total and Spectral Solar Irradiance Sensor (TSIS) Hybrid Solar Reference Spectrum (HSRS) (Coddington et al., 2021) (See section 3.1 for more information) with the Instrument Spectral Response Function (ISRF) of OMS-N. (2) Secondly, the 312-326 nm region is chosen as the retrieval fitting window of the OMS SO<sub>2</sub> column. (3) Thirdly, spectral soft calibration is performed using the absorption peaks and valleys of the solar reference spectrum. (4) Fourthly, the cross sections of SO<sub>2</sub> and O<sub>3</sub> in 312-326 nm are convolved with the ISRF. (5) Fifthly, the Ring spectrum is calculated using the SCIATRAN Radiative Transfer Model (Ročanov et al., 2005). (6) Sixthly, SO<sub>2</sub>, O<sub>3</sub> and Ring cross-sections together with a third-order polynomial are used in the DOAS fitting process to obtain the SCD of OMS SO<sub>2</sub>. (7) Seventhly, the AMF is applied to get vertical column density (VCD). (8) Finally, a specific correction scheme for OMS background offset is applied to effectively reduce along-track stripes and across-track asymmetries in the initial OMS SO<sub>2</sub> retrievals. ...

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Solar Pseudo Transmittance Spectrum (SPTS) atlas. The TSIS-1 HSRS spans 202–2730 nm at 0.01 to ~0.001 nm spectral resolution with uncertainties of 0.3% between 460 and 2365 nm and 1.3% at wavelengths outside that range (Coddington et al., 2021). The TSIS-1 HSRS hybrid solar reference spectrum was convolved with the OMS-N ISRF to match the spectral characteristics of OMS radiance.

### 3.2 Spectral soft calibration

Before the DOAS fitting retrieval, spectral soft calibration was applied to the FY-3F/OMS radiance data. This procedure corrects wavelength shifts caused by instrument drift, temperature fluctuations, radiation effects, and nonlinearities by using known absorption features. It ensures the spectral accuracy and consistency of the OMS radiances, which is essential for accurate SO<sub>2</sub> retrieval and for reducing the impact of calibration-related errors.

The spectral soft calibration is performed using the peaks and valleys of the TSIS-1 HSRS hybrid solar reference spectrum (Van Geffen and Van Oss, 2003; Coddington et al., 2021). The detailed process includes: 1) Selecting the high-resolution hybrid solar reference spectrum (Coddington et al., 2021), and convolving the reference spectrum with the slit function of the FY-3F/OMS instrument; 2) Fitting the ratio of the solar reference spectrum to the observed radiance spectrum with a low-order polynomial to enhance the observed radiance spectrum; 3) For each observed radiance spectrum in the SO<sub>2</sub> fitting window, Gaussian peak-finding is performed to match the peak position of a set of Fraunhofer lines with their corresponding wavelengths. A least-squares method is used to fit the spectral line wavelengths and the peak position number data with a third-order polynomial, generating a spectral calibration equation for each observed pixel. Then the spectral soft calibration of the FY-3F/OMS radiance is realized by using the above spectral calibration equation.

### 3.3 DOAS SCD retrieval

#### 3.3.1 SO<sub>2</sub> fitting window

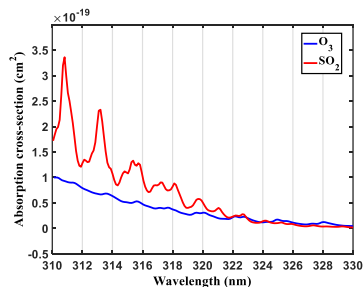


Figure 1: Absorption cross sections of SO<sub>2</sub> and O<sub>3</sub> in the wavelength range 310-330 nm (Bogumil et al., 2003).

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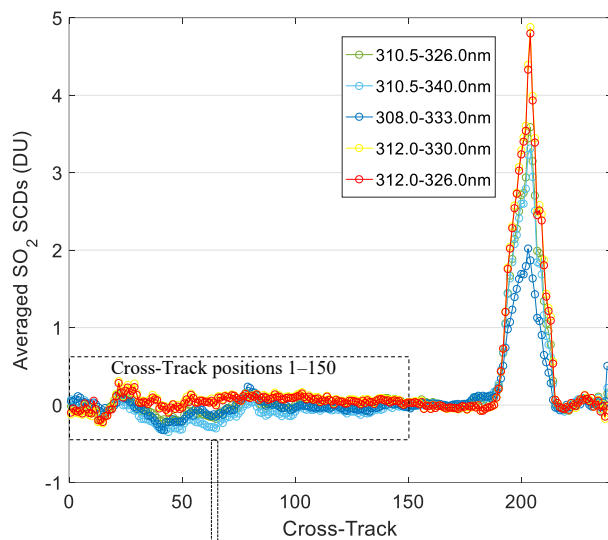
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<u>Fitting window</u>	<u>Standard deviation</u>	<u>Mean value</u>
<u>(nm)</u>	<u>(DU)</u>	<u>(DU)</u>
<u>312-326</u>	<u>0.08</u>	<u>0.04</u>
<u>310.5-326</u>	<u>0.09</u>	<u>-0.03</u>
<u>310.5-340</u>	<u>0.1</u>	<u>-0.1</u>
<u>308-333</u>	<u>0.09</u>	<u>-0.04</u>
<u>312-330</u>	<u>0.09</u>	<u>0.06</u>

**Figure 2:** Row-averaged SO<sub>2</sub> retrievals from OMS rows 700 to 870 of orbit 20240823 1036 by using different spectral fitting windows.

The selection of the retrieval fitting window is crucial for the accuracy of OMS SO<sub>2</sub> retrievals, which significantly affect OMS capability in monitoring SO<sub>2</sub> from volcanic and anthropogenic sources. A suitable fitting window helps to reduce the impact of interfering gases (O<sub>3</sub>), to enhance the SO<sub>2</sub> information content in the satellite signal and to obtain reliable SO<sub>2</sub> results. In this study, the 312-326 nm fitting window was selected for the OMS SO<sub>2</sub> retrievals based on the following considerations.

(1) Shorter wavelengths, despite stronger SO<sub>2</sub> absorption (Fig. 1), suffer from lower SNR and TOA radiance saturation over volcanic plumes, while longer wavelengths introduce more noise due to weaker absorption and O<sub>3</sub> interference, especially under low anthropogenic emissions.

(2) The selected fitting window (312–326 nm) is consistent with the widely used TROPOMI SO<sub>2</sub> product (Theys et al., 2017), facilitating intercomparison and validation of the OMS SO<sub>2</sub> retrievals. For the first results of OMS SO<sub>2</sub> results in this study, we did not adopt multiple fitting windows for different SO<sub>2</sub> concentration conditions as implemented in the TROPOMI product.

(3) Comparisons of SO<sub>2</sub> retrievals from different fitting windows commonly used in published studies—312–326 nm (Theys et al., 2017), 310.5–326 nm (Theys et al., 2021), 310.5–340 nm (Li et al., 2013), 308–333 nm (Yang et al., 2009, 2013), and 312–330 nm (Nowlan et al., 2011)—over the Sundhnúkur volcano and the surrounding clean region on 23 August 2024 (Fig. ) show that the 312–326 nm window has higher SO<sub>2</sub> values within the volcanic plume and lower standard deviations and mean values in the clean region (cross-track positions 1–150). These results demonstrate the suitability of the 312–326 nm fitting window for OMS SO<sub>2</sub> retrievals. The discrete wavelengths (310.8, 311.9, 313.2, and 314.4 nm) used in the Band Residual Difference (BRD) algorithm (Krotkov et al., 2006) were not considered in this study because the OMS SO<sub>2</sub> retrieval is based on DOAS algorithm that employs a hyperspectral UV fitting window. The 300–335 nm fitting window employed in the EISF algorithm (Yang et al., 2010) was also not considered in this study because the OMS VIS band starts at 307 nm, and the OMS UV2 spectral range (300–320 nm) requires further calibration.

### 3.3.2 Ring effect

The Ring effect is an important factor influencing the accuracy of SO<sub>2</sub> retrieval results due to the pronounced filling-in features of the Ring spectrum in the UV region (Fig. 3). It redistributes photon energy and leads to the filling-in of Fraunhofer and atmospheric absorption lines (Sioris and Evans, 1999; Fish and Jones, 1995; Chance and Spurr, 1997; Vountas et al., 1998). For OMS SO<sub>2</sub> column retrievals using the DOAS method, the Ring effect is considered as a pseudo-absorption effect, and the Ring spectrum calculated using the SCIATRAN radiative transfer model (Rozanov et al., 2005) is included as a pseudo-absorber in the spectral fitting process, as shown in Equation (1).

$$-\ln \frac{\pi \cdot I(\lambda)}{F(\lambda) \cdot \cos(SZA)} = \sigma_{\text{SO}_2}(\lambda) \times \text{SCD}_{\text{SO}_2} + \sigma_{\text{O}_3}(\lambda) \times \text{SCD}_{\text{O}_3} + \sigma_{\text{Ring}}(\lambda) \times C_{\text{Ring}} + P(\lambda) + E(\lambda) \quad (\text{Eq. 1})$$

Where  $I(\lambda)$  and  $F(\lambda)$  are the satellite-observed radiance and the solar reference spectrum convolved with the OMS ISRF,  $SZA$  is the Solar Zenith Angle,  $\sigma_{\text{SO}_2}(\lambda)$  and  $\sigma_{\text{O}_3}(\lambda)$  are the absorption cross-section of SO<sub>2</sub> and O<sub>3</sub>,  $\text{SCD}_{\text{SO}_2}$  and  $\text{SCD}_{\text{O}_3}$  are the slant column density of SO<sub>2</sub> and O<sub>3</sub>,  $\sigma_{\text{Ring}}(\lambda)$  is the Ring spectrum calculated using the SCIATRAN model and convolved with the OMS ISRF,  $C_{\text{Ring}}$  is the Ring absorption coefficient determined by the fitting,  $P(\lambda)$  is a low-order polynomial, and  $E(\lambda)$  is the error term.

Note that in this study a fixed Ring spectrum calculated using the SCIATRAN model under typical atmospheric and surface conditions and observational geometry ( $SZA=30^\circ$ , Viewing Zenith Angle (VZA)= $0^\circ$ , Relative Azimuth Angle (RAA)= $0^\circ$ ,

surface reflectance (AS)=0.05, surface height above sea level (HS) (also referred to as terrain height)=0 km, ozone column=275 DU, clear sky) is used in the DOAS fitting for all OMS measurements. Variations of the Ring spectrum due to different atmospheric conditions and viewing geometries are not considered, since applying the Ring lookup table would be computationally costly and its impact on OMS SO<sub>2</sub> SCD retrievals is limited. A detailed error analysis of this fixed Ring approach is discussed in Section 5.1.3.

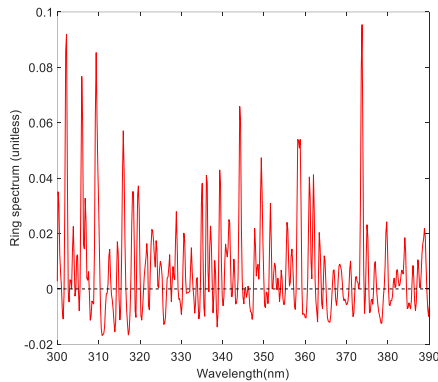


Figure 3: Ring spectrum calculated with the SCIATRAN model, convolved with the OMS nadir ISRF. SCIATRAN forward settings are SZA=30°, VZA=0°, RAA=0°, Surface albedo=0.05, Ozone column=275 DU, Clear sky.

### 3.3.3 Spectral fitting

The retrieval of the FY-3F/OMS SO<sub>2</sub> SCD is primarily based on the classical DOAS theory (Platt and Stutz, 2008). It utilizes Beer-Lambert's law and the satellite hyperspectral radiance observations in the UV fitting window to derive the SO<sub>2</sub> SCD along the entire photon path. First, the absorption cross-section of SO<sub>2</sub> and O<sub>3</sub>, measured under specific laboratory conditions with a higher spectral resolution and different sampling points than those of OMS observations, are convolved with the OMS ISRF to match the spectral resolution of the OMS instrument. Secondly, atmospheric extinction is divided into two components: a fast-varying part with wavelength, typically associated with narrow absorption features of SO<sub>2</sub> and O<sub>3</sub>, and a slow-varying part with wavelength, related to broad spectral features of absorption and atmospheric scattering processes such as Rayleigh and Mie scattering. A low-order polynomial is used to remove the slow-varying components, while preserving the fast-varying part related to SO<sub>2</sub> and O<sub>3</sub> absorption. Finally, the slow-varying part of satellite-observed TOA reflectance (the ratio of L1 radiance to irradiance data) are removed by subtracting a low-order polynomial, and the atmospheric SO<sub>2</sub> SCD is obtained through least-squares fitting.

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(2) in this study, (3) Comparisons between SO<sub>2</sub> retrievals from different fitting windows used in the literature (312-326nm (Theys et al., 2017), 310.5-326nm(Theys et al., 2021), 310.5-340nm(Li et al., 2013), 308-333nm (Yang et al., 2009; Yang et al., 2013), 312-330nm (Nowlan et al., 2011)) over the Sundhnúkur volcano and its surrounding clean region for August 23, 2024 (Fig. 2) show that the retrieval results from the 312-326 nm fitting window have higher SO<sub>2</sub> values in the volcanic region, and exhibit lower standard deviations and mean values in the clean regions (cross-track positions 1-150). 也就是说, demonstrate the advantage 可行性 of the 312-326 nm fitting window for OMS SO<sub>2</sub> retrievals. The four discrete retrieval wavelengths (310.8, 311.9, 313.2, and 314.4 nm) used by Band Residual Difference (BRD) algorithm (Krotkov et al., 2006) are not included in this study due to the OMS SO<sub>2</sub> DOAS retrieval using a continuous UV fitting window for SO<sub>2</sub> retrieval. The 300-335 nm fitting window used by the ELSF algorithm (Yang et al., 2010) also was not included in this study because the OMS VIS spectral band starts from 307 nm and the OMS UV2 spectral range from 300 nm to 320 nm requires further calibration.

In this study, the 312-326 nm fitting window was chosen for the SO<sub>2</sub> retrieval from OMS observations. This is mainly based on the following considerations:

(1) Firstly, in the wavelength range 310-330 nm, although SO<sub>2</sub> has stronger absorption at shorter wavelengths (Fig. 1) which would make it preferable, satellite measurements at shorter wavelengths have lower SNR, and in the case of volcanic SO<sub>2</sub> emission, the TOA reflected radiances are prone to saturation which leads to underestimation of volcanic SO<sub>2</sub>. Therefore, it is not appropriate to select the fitting window with the strongest SO<sub>2</sub> absorption for SO<sub>2</sub> retrieval.

(2) Secondly, longer UV wavelengths, due to the weaker absorption of SO<sub>2</sub>, tend to introduce more noise into the retrieval of the SO<sub>2</sub> column. This is because the weaker absorption may make it more difficult to accurately distinguish the SO<sub>2</sub> absorption information from background noise and interference of O<sub>3</sub> absorption, especially in the case of low SO<sub>2</sub> emissions from anthropogenic sources.

(3) Thirdly, selecting the 312-326 nm fitting window makes the OMS SO<sub>2</sub> product consistent with the widely used TROPOMI SO<sub>2</sub> product (Theys et al., 2017). However, in this study, we did not adopt a strategy with multiple fitting windows for different SO<sub>2</sub> concentration conditions as is used in the TROPOMI product.

(4) Finally, in order to demonstrate the advantage of the 312-326 nm fitting window for OMS SO<sub>2</sub> retrievals, comparisons were conducted between SO<sub>2</sub> retrievals from different fitting windows over the Sundhnúkur volcano and its surrounding clean region for August 23, 2024 (Figs. 2, 3, and 4). Note that negative values often appear in SO<sub>2</sub> retrievals, and small negative values can indicate low SO<sub>2</sub> emissions in clean areas. In this study, all SO<sub>2</sub> retrievals greater than -10 DU are selected for comparison to exclude obvious outliers. The details of the comparisons are described below.

The main fitting windows and retrieval algorithms used in the literature for SO<sub>2</sub> retrievals based on ultraviolet hyperspectral satellite measurements are listed in Table 2. The OMS SO<sub>2</sub> columns retrieved using these different fitting windows are shown in Figs. 2, 3, and 4. Note that due to the DOAS algorithm generally using a continuous UV fitting window for SO<sub>2</sub> retrieval, the OMS SO<sub>2</sub> results from BRD four discrete wavelengths (310.8, 311.9, 313.2, and 314.4 nm) at absorption peak and valley (Krotkov et al., 2006) are not included in this study. It also should be noted that, since the OMS VIS spect...

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**Table 2. Parameter settings for the retrieval of FY-3F/OMS SO<sub>2</sub> SCD**

Parameter	FY-3F/OMS SO <sub>2</sub> DOAS settings
Retrieval fitting window	312–326 nm
Solar irradiance	TSIS-1 HSRS hybrid solar reference spectrum (Coddington et al., 2021)
Cross-sections	SO <sub>2</sub> 273K (Bogumil et al., 2003) O <sub>3</sub> 223K (Bogumil et al., 2003)
Ring effect	Ring spectrum calculated using the SCIATRAN model at SZA=30°, VZA=0°, RAA=0°, AS=0.05, Clear sky (Rozanov et al., 2005)
Polynomial	3 <sup>th</sup> order
Background offset correction	Iterative and sliding correction scheme

### 3.4 AMF

The reflected radiance detected by the satellite instrument contains information of trace gases integrated along the slant observation path. From the reflected radiance and above DOAS spectral fitting, the SO<sub>2</sub> SCD can be derived; however, the SCD is not suitable for the application of satellite-derived SO<sub>2</sub> in monitoring global climate change and air pollution, as it represents the SO<sub>2</sub> column along the slant path, which is influenced by the observation geometry and atmospheric conditions. The SCD can be converted to VCD using AMF=SCD/VCD (Palmer et al., 2001), which represents the relative length of the mean slant path at a certain wavelength for photons interacting with a certain absorber in the atmosphere relative to the vertical path (Lorente et al., 2017).

The AMF can be expressed as a function of these parameters:

$$AMF = f(SZA, VZA, RAA, AS, HS, S(z), O_3, \lambda, \text{clouds, aerosols}) \quad (\text{Eq. 2})$$

Where AS is the surface reflectance, HS is the terrain height, S(z) represents the SO<sub>2</sub> vertical profile shape, O<sub>3</sub> is total ozone column. In practice, the AMF is typically computed as the weighted average of altitude-dependent Box-AMFs (equivalent to scattering weights) across all layers, with the weights determined by the SO<sub>2</sub> distribution in each layer (Eq. 3) (Chen et al., 2009; Wagner et al., 2007; Palmer et al., 2001; Boersma et al., 2004):

$$AMF = \sum_i \text{Box-AMF}_i \times \frac{c_i \Delta h_i}{\sum_j c_j \Delta h_j} \quad (\text{Eq. 3})$$

Where c<sub>i</sub> represents the SO<sub>2</sub> number density in the i-th layer, and Δh<sub>i</sub> denotes the thickness of that layer. Box-AMFs quantify the contribution of each atmospheric layer to the total AMF and allows for flexible updates of AMF with new SO<sub>2</sub> profiles, eliminating the procedure of rebuilding the AMF lookup table (LUT).

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### Deleted: 3.4 Background offset correction

The retrieval accuracy of SO<sub>2</sub> columns from satellite measurements is usually affected by spectral and radiometric calibration errors, which are difficult to remove from L1 radiance data and result in systematic biases in the retrieval results, such as along-track stripes and cross-track asymmetry (Boersma et al., 2004). In addition, due to the low SNR of measurements in the fitting window, the weak SO<sub>2</sub> absorption information included in the TOA reflected radiance, and the interference from strong O<sub>3</sub> absorption in the fitting window, the OMS SO<sub>2</sub> retrievals tend to be systematically overestimated or underestimated over the whole orbit. These systematic biases in the retrieval results of SO<sub>2</sub> columns are mixed with the absorption information of SO<sub>2</sub> and limit the applicability of the OMS SO<sub>2</sub> product. Therefore, it is necessary to apply a background offset correction to reduce these systematic biases in the retrieved SO<sub>2</sub> columns. The reference region method (Khokhar et al., 2005; Richter et al., 2006) was used to correct the background offsets, which are latitude-dependent and related to the cross-track position. This method selects retrieval values over a reference region (e.g., clean oceanic Pacific regions, assumed to be areas with no SO<sub>2</sub>) as the background area. The SO<sub>2</sub> retrievals are then adjusted by subtracting the background offsets of the same latitude over the ocean. Yang proposed the sliding median correction method (Yang et al., 2007) and applied it to the OMI SO<sub>2</sub> product. This method performs averaged sampling within a sliding window centered on the pixel (selecting pixels with values less than 2 DU) to get background offsets for each row of pixels. With the sliding window method, the cross-track and along-track biases varying with time and location can be effectively eliminated.

For OMS SO<sub>2</sub> retrievals, based on the above background offset correction methods, we developed an improved iterative sliding correction scheme to avoid seam problems due to discontinuous integration times within the same orbit. The details of the background offset correction used for OMS SO<sub>2</sub> retrievals are as follows.

(1) Firstly, based on the integration time of FY3F/OMS L1 data, the orbital data is divided into several data blocks corresponding to different integration times. For each data block, the mean vector (V0) at each cross-track position is estimated using all valid pixels within the block (i.e., pixels with normal L1 data, as indicated by the L1 QA quality flag). Each scan line within the data block is processed by subtracting V0 from the SO<sub>2</sub> retrievals of each scan line to obtain the initially corrected SO<sub>2</sub> columns.

(2) Secondly, based on the initially corrected SO<sub>2</sub> columns, the predefined SO<sub>2</sub> threshold (2 DU), and the sliding window, the mean vector V1 for cross-track positions within each sliding window is estimated. The initially corrected SO<sub>2</sub> columns are then processed by subtracting V1 to obtain the double-corrected SO<sub>2</sub> columns. Note that the size of the sliding window varies with the satellite's spatial resolution. In this study, for the FY3F/OMS with nadir resolution...

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In this study, OMS SO<sub>2</sub> AMFs were calculated using Box-AMFs derived from SCIATRAN and SO<sub>2</sub> vertical profiles from the Goddard Earth Observing System Composition Forecast (GEOS-CF) system (Fahrland et al., 2020) (Data source: <https://portal.nccs.nasa.gov/datashare/gmao/geos-cf>). The GEOS-CF system combines the GEOS weather analysis and forecasting system with the GEOS-Chem chemistry module (Keller et al., 2021) to provide detailed chemical analyses of a wide range of air pollutants, including O<sub>3</sub>, NO<sub>2</sub>, SO<sub>2</sub>, and PM<sub>2.5</sub>. The GEOS-CF SO<sub>2</sub> vertical profiles, with a horizontal resolution of 0.25° × 0.25°, a temporal resolution of 1 hour, and 72 vertical model layers extending up to 0.01 hPa, were temporally matched to the OMS overpass time and spatially interpolated to the center of each OMS pixel. The profiles were normalized and used as weighting functions in the AMF calculation.

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To improve computational efficiency, a cloud-free Box-AMF LUT was built using SCIATRAN, considering six variables: SZA, VZA, RAA, AS, HS, and O<sub>3</sub> column. The detailed values for each variable are listed in Table 3. Although Box-AMFs are wavelength-dependent, the LUT in this study was calculated at 320 nm, approximately at the center of the OMS SO<sub>2</sub> retrieval window (312–326 nm). For each OMS pixel, Box-AMF values were obtained by multi-dimensional interpolation within the LUT according to the corresponding observational geometry (SZA, VZA, and RAA) and atmospheric and surface conditions (AS, HS, and O<sub>3</sub>). The observational geometry parameters and surface height were directly obtained from the OMS L1 radiance product. The corresponding surface reflectance was interpolated from the OMI surface reflectance climatology (Kleipool et al., 2008). The total ozone column used for LUT interpolation was obtained from the corresponding OMS ozone product (Xu et al., 2025). Due to the current unavailability of synchronized and reliable OMS cloud and aerosol products, the effects of clouds and aerosol on SO<sub>2</sub> retrievals were not considered in this study. Consequently, the AMFs for all OMS pixels were calculated using the cloud-free Box-AMF LUT. Section 5.2 of this study provides a detailed description of the AMF error analysis.

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**Table 3. Values of the six variables used in the cloud-free Box-AMF LUT**

Variable	Values
SZA (°)	0, 9.3, 21.2, 32.9, 44.2, 54.9, 64.8, 73.5, 80.8, 86.1
VZA (°)	0, 9.3, 21.2, 32.9, 44.2, 54.9, 64.8, 73.5
RAA (°)	0, 30, 60, 90, 120, 150, 180
AS	0, 0.01, 0.025, 0.05, 0.075, 0.1, 0.15, 0.2, 0.25, 0.325, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1
HS (km)	0, 0.5, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12
O <sub>3</sub> column (DU)	75, 125, 175, 225, 275, 325, 375, 425, 475, 525, 575

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590 **3.5 Background offset correction**

The retrieval accuracy of SO<sub>2</sub> columns from FY-3F/OMS is affected by spectral and radiometric calibration errors, which are difficult to remove from OMS L1 radiance data and result in systematic biases in the retrieval results, such as along-track stripes and cross-track asymmetries (Boersma et al., 2004). The TSIS-1 HSRS hybrid solar reference spectrum used in OMS SO<sub>2</sub> retrievals does not contain instrument-related characteristics, meaning that certain calibration errors in the radiance data cannot be cancelled out during the DOAS fitting process. This may further contribute to systematic biases in the retrieved OMS SO<sub>2</sub> columns. In addition, due to the low SNR of measurements in the fitting window, the weak SO<sub>2</sub> absorption information included in the TOA reflected radiance, and the interference from strong O<sub>3</sub> absorption in the fitting window, the OMS SO<sub>2</sub> retrievals tend to be systematically overestimated or underestimated over the whole orbit. These systematic biases in the retrieval results of SO<sub>2</sub> columns are mixed with the absorption information of SO<sub>2</sub> and limit the applicability of the OMS SO<sub>2</sub> product. Therefore, it is necessary to apply a background offset correction to reduce these systematic biases in the retrieved SO<sub>2</sub> columns. The reference region method (Khokhar et al., 2005; Richter et al., 2006) was used to correct the background offsets, which are latitude-dependent and related to the cross-track position. This method selects retrieval values over a reference region (e.g., clean oceanic Pacific regions, assumed to be areas with no SO<sub>2</sub>) as the background area. The SO<sub>2</sub> retrievals are then adjusted by subtracting the background offsets of the same latitude over the ocean. Yang proposed the sliding median correction method (Yang et al., 2007) and applied it to the OMI SO<sub>2</sub> product. This method performs averaged sampling within a sliding window centered on the pixel (selecting pixels with values less than 2 DU) to get background offsets for each row of pixels. With the sliding window method, the cross-track and along-track biases varying with time and location can be effectively eliminated.

For OMS SO<sub>2</sub> retrievals, based on the above background offset correction methods, we developed an improved iterative sliding correction scheme to avoid seam problems due to discontinuous integration times within the same orbit. The details of the background offset correction used for OMS SO<sub>2</sub> retrievals are as follows.

(1) Firstly, based on the integration time of FY-3F/OMS L1 data, the orbital data is divided into several data blocks corresponding to different integration times. For each data block, the mean vector ( $V_0$ ) at each cross-track position is estimated using all valid pixels within the block (i.e., pixels with normal L1 data, as indicated by the L1 QA quality flag). Each scan line within the data block is processed by subtracting  $V_0$  from the SO<sub>2</sub> retrievals of each scan line to obtain the initially corrected SO<sub>2</sub> columns.

(2) Secondly, based on the initially corrected SO<sub>2</sub> columns, the predefined SO<sub>2</sub> threshold (2 DU), and the sliding window, the mean vector  $V_1$  for cross-track positions within each sliding window is estimated. The initially corrected SO<sub>2</sub> columns are then processed by subtracting  $V_1$  to obtain the double-corrected SO<sub>2</sub> columns. Note that the size of the sliding window varies with the satellite's spatial resolution. In this study, for the FY-3F/OMS with nadir resolution of 7 km×7 km, the sliding window is set to 200 scan lines. It is worth noting that there is a trade-off between the size of the sliding window and

the effectiveness of the offset correction: too big a window might result in poor offset correction, while too small a sliding window might lead to reduction of the SO<sub>2</sub> information contained in the satellite measurements.

625 (3) Finally, based on the double-corrected SO<sub>2</sub> results, the predefined SO<sub>2</sub> threshold, and the sliding window, an iterative procedure is performed until the relative deviation between the results of the two consecutive corrections is less than or equal to 5%.

#### 4 Comparison of OMS SO<sub>2</sub> columns with TROPOMI observations

630 Based on the FY-3F/OMS L1 measurements and the retrieval scheme outlined in section 3, global SO<sub>2</sub> columns from FY-3F/OMS were retrieved and applied to monitor the SO<sub>2</sub> emissions from volcanic and anthropogenic activities. Evaluating the accuracy of OMS SO<sub>2</sub> retrievals is challenging, as it is difficult to obtain synchronous and high-quality ground-based or airborne measurements for the validation of OMS SO<sub>2</sub> retrievals. Therefore, in this study, due to its high spatial and spectral resolution in the UV-VIS band and its common use in global SO<sub>2</sub> monitoring, the TROPOMI SO<sub>2</sub> total column product was selected as reference to evaluate the accuracy of OMS SO<sub>2</sub> retrievals (Theys et al., 2019; Wang et al., 2022; Theys et al., 2017; Cofano et al., 2021; Corradino et al., 2024; Fioletov et al., 2020). It should be noted that, in the comparison between OMS and TROPOMI SO<sub>2</sub> results, no filtering for cloud or large SZA was applied to the OMS SO<sub>2</sub> data. Instead, all OMS SO<sub>2</sub> retrievals greater than -10 DU were selected for the comparison, since negative values often appear in SO<sub>2</sub> retrievals from most instruments (e.g., OMI, GOME-2, and TROPOMI), and small negative values can indicate low SO<sub>2</sub> emissions in clean areas (Theys et al., 2013; Fioletov et al., 2020).

640 TROPOMI has a local overpass time of approximately 13:30, a spatial resolution of 5.5 km×3.5 km for SO<sub>2</sub> and provides daily global coverage with about 14 orbits per day. Two TROPOMI SO<sub>2</sub> products derived from different retrieval algorithms are used for comparison in this study: one is the TROPOMI offline L2 orbital SO<sub>2</sub> product from the DOAS algorithm (hereafter referred to as TROPOMI DOAS or TROPOMI-D) (Data source: <https://browser.dataspace.copernicus.eu/>), and the other is the TROPOMI L3 grid Planetary Boundary Layer (PBL) and 7km SO<sub>2</sub> product from the COBRA algorithm (hereafter referred to as TROPOMI COBRA or TROPOMI-C) (Data source: <https://data-portal.s5p-pal.com/products/so2cbr.html>). The TROPOMI DOAS SO<sub>2</sub> retrieval uses multiple spectral windows, including 312–326 nm, 325–335 nm, and 360–390 nm (Theys et al., 2017), which helps mitigate saturation effects under volcanic eruptions, whereas the TROPOMI COBRA algorithm uses 310.5–326 nm as the retrieval window, where SO<sub>2</sub> absorption is relatively strong. The TROPOMI COBRA SO<sub>2</sub> product was developed by Royal Belgian Institute for Space Aeronomy (BIRA), and reduces significantly both the noise and biases present in the current TROPOMI operational DOAS SO<sub>2</sub> retrievals (Theys et al., 2021). The TROPOMI COBRA L3 grid product (0.022°×0.022° equal latitude-longitude grid) was generated using the HARP gridding tool from L2 data applying a Quality Assurance (QA) filter (QA>0.5) to remove low quality data. This quality filtering may leads to some gaps in the COBRA data.

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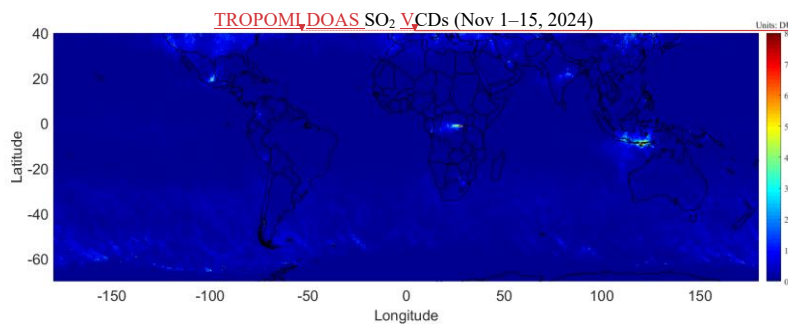
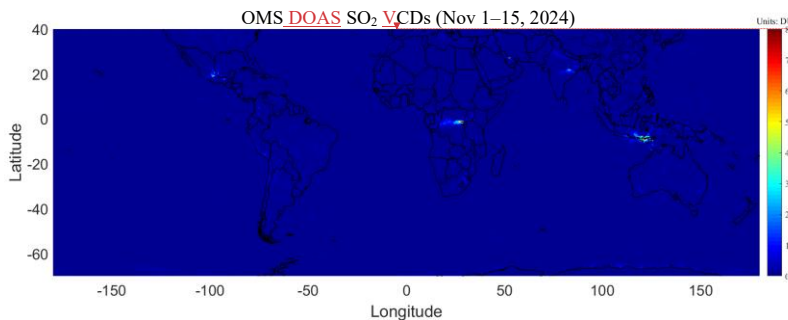
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Figure 4 shows the 15-days averaged global SO<sub>2</sub> VCDs from OMS, TROPOMI DOAS and TROPOMI COBRA for November 1–15, 2024. OMS DOAS SO<sub>2</sub> VCDs were averaged using pixels with SO<sub>2</sub> column greater than -10 DU, while TROPOMI DOAS VCDs used pixels with QA > 0.5. Overall, the OMS, TROPOMI DOAS and TROPOMI COBRA datasets exhibit generally consistent spatial distributions, clearly identifying the major global SO<sub>2</sub> emission hotspots. Minor differences between the datasets can be attributed to variations in observational geometry, overpass time, and algorithmic processing. Further comparisons based on individual orbits are presented in Sections 4.1, 4.2, and 4.3. Based on these comparisons, the performance of OMS SO<sub>2</sub> retrievals was evaluated over clean oceanic regions, volcanic eruption regions, and anthropogenic emission regions, as marked by the red boxes in the Fig. 5.



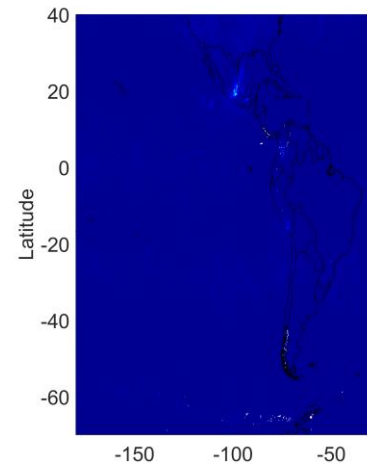
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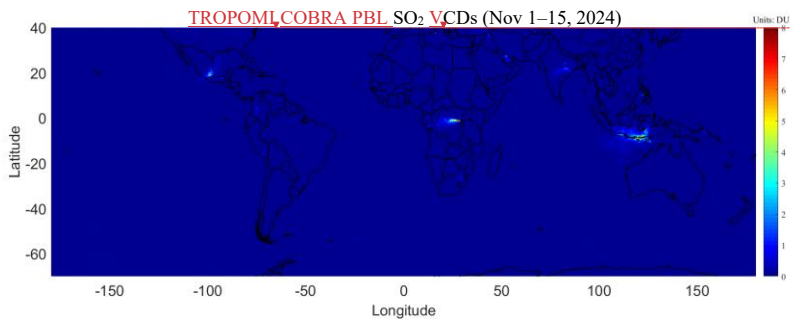
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715 **Figure 4: Global maps of averaged SO<sub>2</sub> VCDs from OMS, TROPOMI DOAS and TROPOMI COBRA for November 1–15, 2024, 0.2°×0.2° equal latitude-longitude grid. Note that the TROPOMI DOAS SO<sub>2</sub> VCDs are obtained from the product variable 'sulfurdioxide total vertical column', and only pixels with QA > 0.5 are used.**

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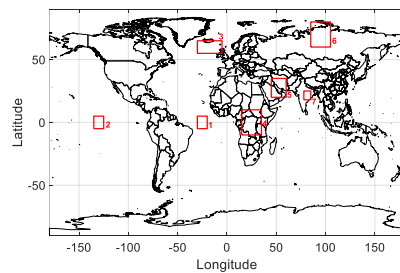
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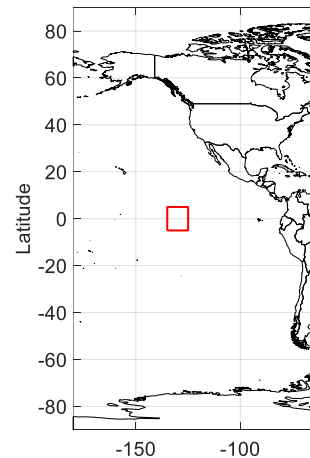
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720 **Figure 5: Regions selected for the comparison of OMS and TROPOMI SO<sub>2</sub> columns. Regions 1 and 2 represent clean oceanic areas, regions 3 and 4 correspond to volcanic eruption areas, and regions 5–7 represent anthropogenic emission areas.**

#### 4.1 Comparison over clean oceanic regions

Ideally, the retrieved SO<sub>2</sub> values from satellite observations in clean regions should be close to zero. The scatter of SO<sub>2</sub> columns in clean regions can reflect the reliability and stability of the satellite data and the retrieval algorithm (Krotkov et al., 2008). In this study, two clean oceanic regions, where SO<sub>2</sub> emissions are extremely low and assumed to be zero, were selected as the case studies to compare and evaluate the precision of FY-3F/OMS SO<sub>2</sub> retrievals. One is the area of latitude from 5°S to 5°N and longitude from 30°W to 20°W (Region 1 in Fig. 5), and the other is the area of latitude from 5°S to 5°N and longitude from 135°W to 125°W (Region 2 in Fig. 5). Due to the geolocation differences between OMS and TROPOMI orbits, the orbital pixels of OMS and TROPOMI DOAS and TROPOMI COBRA SO<sub>2</sub> product over the two clean oceanic regions were resampled to 0.15°×0.15° equal latitude-longitude grid for comparison. As suggested in the TROPOMI



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README file, only pixels with QA > 0.5 were used for the TROPOMI DOAS SO<sub>2</sub> product [in this section](#). For the cases of clean oceanic regions, TROPOMI COBRA L3 grid PBL SO<sub>2</sub> products were used instead of the COBRA 7km product.

[As shown in Figs. 6, 7, 8, and 9, the SO<sub>2</sub> columns retrieved from both OMS and TROPOMI over Region 1 and Region 2 are generally low and close to zero, and they approximately follow a normal distribution centered around 0, with most values concentrated between -2 DU and 2 DU. However, there are small differences between OMS and TROPOMI SO<sub>2</sub> over clean oceanic regions, which become larger as the pixels approach the edge of the orbit, where retrieval uncertainties are larger. For Region 1, the standard deviations of OMS, TROPOMI DOAS and TROPOMI COBRA SO<sub>2</sub> columns are 0.1537 DU, 0.2493 DU and 0.1156 DU on August 23, 2024, and 0.1672 DU, 0.3934 DU and 0.1865 DU on November 15, 2024, respectively. For Region 2, the corresponding standard deviations are 0.1539 DU, 0.2636 DU and 0.1035 DU on August 23, 2024, and 0.1284 DU, 0.3595 DU and 0.1615 DU on November 15, 2024, respectively. Compared with TROPOMI DOAS SO<sub>2</sub> results, both TROPOMI COBRA and OMS DOAS SO<sub>2</sub> results show lower standard deviations and are closer to zero over Regions 1 and 2. The differences between OMS and TROPOMI SO<sub>2</sub> columns may be primarily related to differences in local overpass times, observation angles, L1 and L2 processing algorithms.](#)

[Overall, comparisons from different dates and different clean oceanic regions indicate that FY-3F/OMS SO<sub>2</sub> retrievals have a reliable precision of approximately 0.15 DU over low-emission regions, and the data quality is relatively stable over time. It is worth noting that the retrieval errors for both OMS and TROPOMI are relatively large at the edges of the orbit, which is likely due to fewer valid pixels in these regions, resulting in larger standard deviations; thus, these pixels should be used with caution.](#)

**Deleted:** For OMS SO<sub>2</sub> retrievals, all pixels with SO<sub>2</sub> column greater than -10 DU are selected for comparison.

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Region 1 (ocean area), 20240823

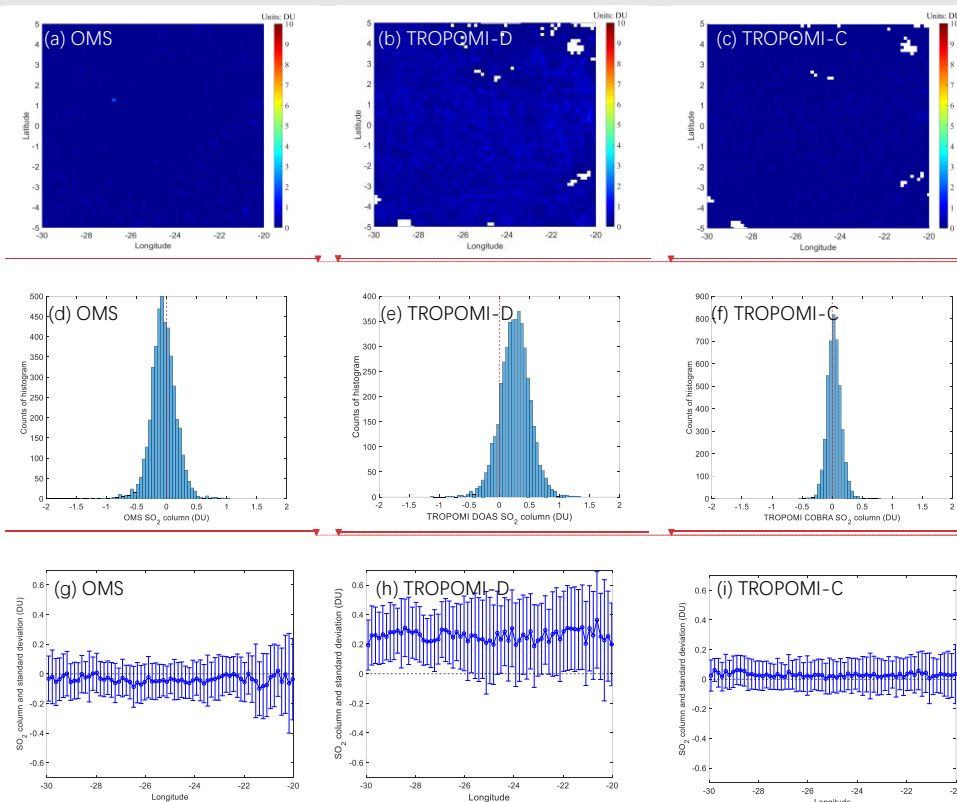
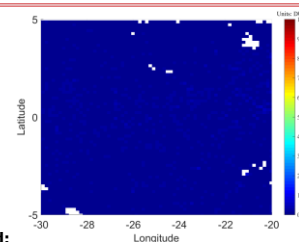
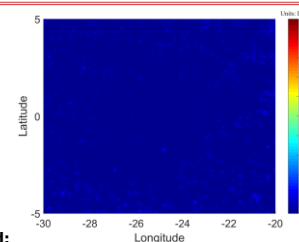


Figure 6: SO<sub>2</sub> retrievals over clean oceanic area (latitude from 5°S to 5°N and longitude from 30°W to 20°W, **Region 1**) on August 23, 2024. (a, b, c) Spatial distribution of resampled **FY-3F/OMS**, TROPOMI DOAS (TROPOMI-D) and TROPOMI COBRA (TROPOMI-C) PBL SO<sub>2</sub> columns over **Region 1**; (b, d, f) Histogram of resampled OMS, TROPOMI DOAS and TROPOMI COBRA PBL SO<sub>2</sub> columns over **Region 1**; (g, h, i) Variation and standard deviations of the latitude-averaged SO<sub>2</sub> columns over **Region 1**. Note that OMS pixels with SO<sub>2</sub> column less than -10 DU and TROPOMI DOAS pixels with QA < 0.5 are assigned the value of -9999 and are not shown in the figures. The missing pixels in Figures **b** and **c** are due to quality filtering applied to TROPOMI data.

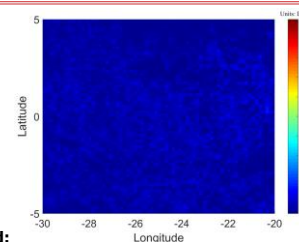
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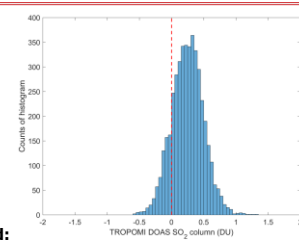
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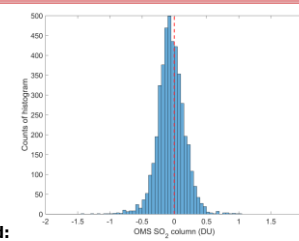
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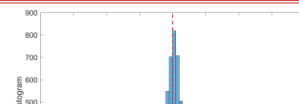
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Region 1 (ocean area), 20241115

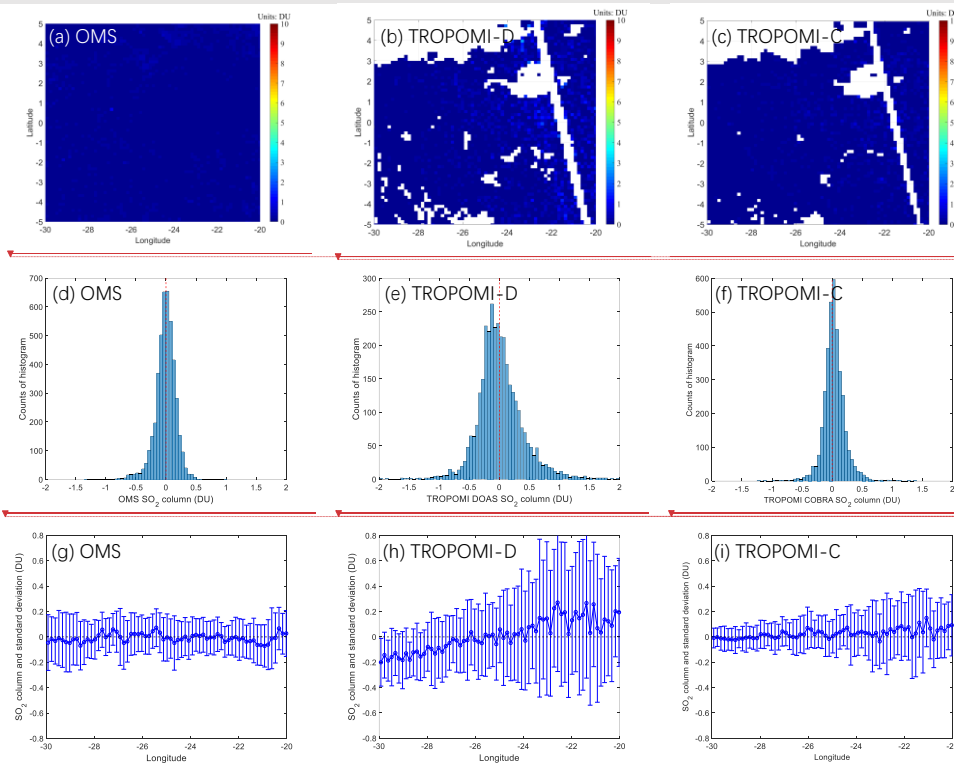
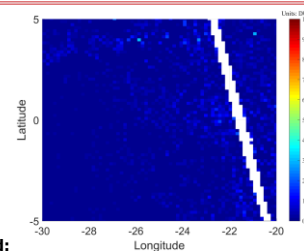
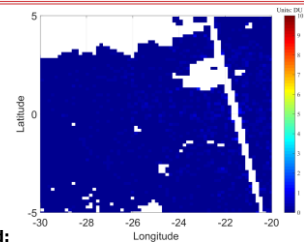


Figure 7: As Fig. 6, but for November 15, 2024. The missing pixels in Figure b and c are due to the gap between the two TROPOMI orbits, and quality filtering applied to TROPOMI data.

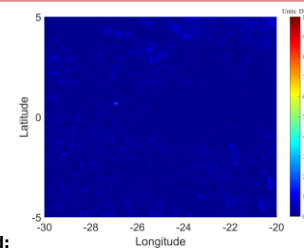
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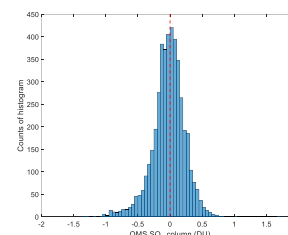
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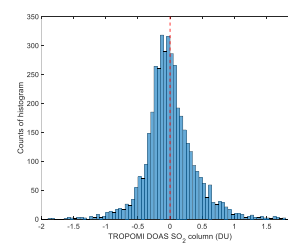
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Region 2 (ocean area), 20240823

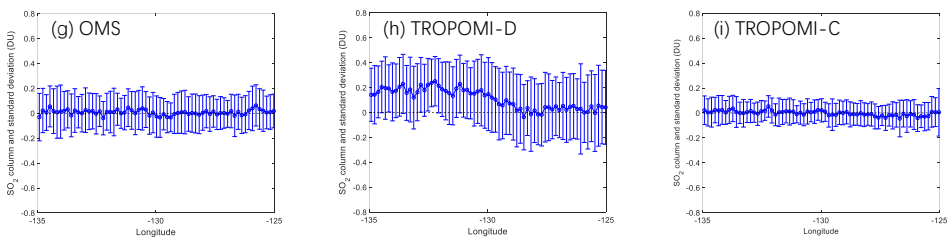
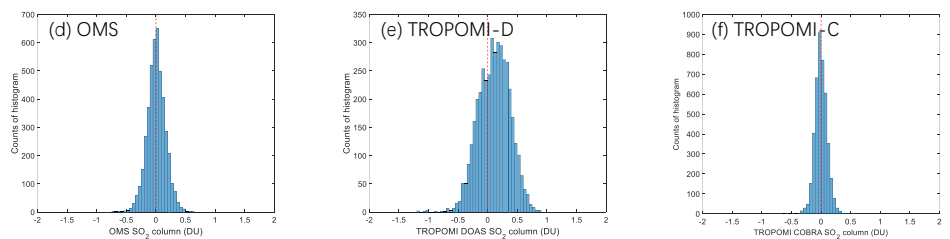
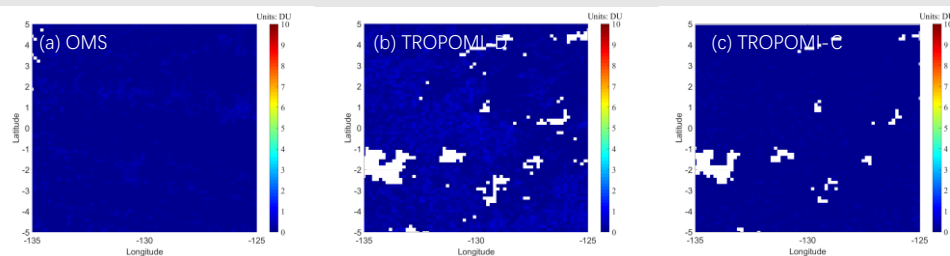
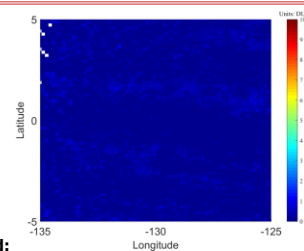
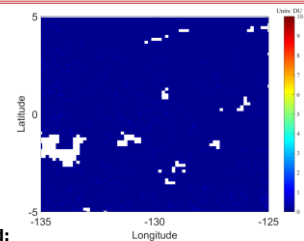


Figure 8: As Fig. 6, but for **Region 2** (latitude from 5°S to 5°N and longitude from 135°W to 125°W). The missing pixels in the Figure a are caused by low spatial resolution at the edges of the orbits, and the missing pixels in the Figures b and c are caused by the quality filtering applied to TROPOMI data.

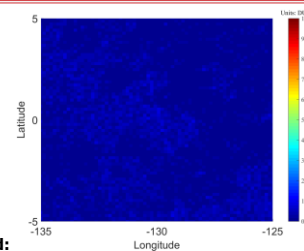
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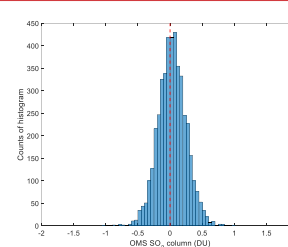
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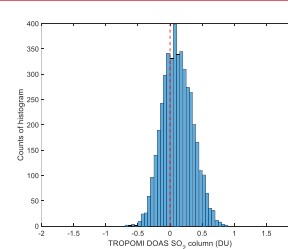
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Region 2 (ocean area), 20241115

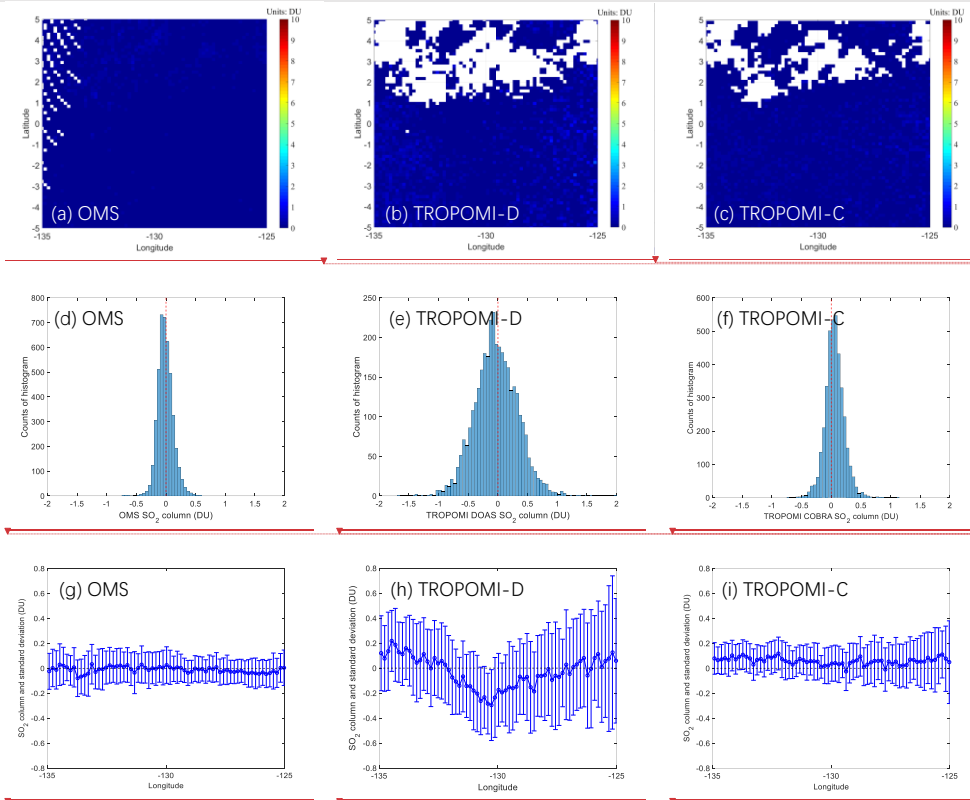


Figure 9: As Fig. 8 but for November 15, 2024. The missing pixels in the Figure a are caused by low spatial resolution at the edges of the orbits, and the missing pixels in the Figures b and c are caused by the quality filtering applied to TROPOMI data.

4.2 Comparison over volcanic eruptions

The massive amounts of SO<sub>2</sub> released over a short period during volcanic eruptions, as well as their long-distance transport (McCormick et al., 1995) but also pose risks to aviation in the tropopause or stratosphere (Miller and Casadevall, 2000). Through the

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comparison in volcanic regions, the capability of OMS SO<sub>2</sub> retrievals at large columns can be evaluated. In this section, we took the eruptions of Sundhnúkur volcano (Region 3 in Fig. 5) and Nyamuragira volcano (Region 4 in Fig. 5) as case studies for comparing FY-3F/OMS SO<sub>2</sub> with TROPOMI DOAS and TROPOMI COBRA 7km SO<sub>2</sub> results. To present the SO<sub>2</sub> maps of OMS and TROPOMI DOAS more clearly, the resampling scheme in section 4.1 was not used in section 4.2. For TROPOMI DOAS, we used all pixels from the TROPOMI DOAS SO<sub>2</sub> product instead of applying QA > 0.5 to filter the high-quality pixels when comparing with the OMS SO<sub>2</sub> results. The reason is that after applying the QA > 0.5 filter, a lot of high SO<sub>2</sub> pixels in TROPOMI DOAS over volcanic regions would be missing (not shown here), making it difficult to compare with OMS SO<sub>2</sub> results. In this section, TROPOMI COBRA L3 grid 7km SO<sub>2</sub> products were used instead of PBL products.

The Sundhnúkur volcano (Region 3 in Fig. 5) is the first case study for comparing FY-3F/OMS SO<sub>2</sub> with TROPOMI DOAS and TROPOMI COBRA 7km SO<sub>2</sub> results over a volcanic eruption. On August 22, 2024, Sundhnúkur volcano within the Reykjanes volcanic system began erupting and continued to emit SO<sub>2</sub> for approximately 14 days (<https://volcano.si.edu/>).

The eruption created a fissure approximately 3.9 km long, with lava and smoke reaching a height of about 1 km. The region of latitude from 55°N to 65°N and longitude from 30°W to 5°W was selected as the study area for the Sundhnúkur volcano. There are two OMS orbits (20240823\_1036 and 20240823\_1217) (Format: YYYYMMDD\_HHMM, UTC time of the first scan line) overpassing the Sundhnúkur volcano region on August 23, 2024. For the OMS orbit 20240823\_1217, most of the pixels covering the volcanic region are near the edge of the orbit where the measurement noise tends to be higher. For TROPOMI DOAS, although two orbits (20240823T125304 and 20240823T111134) (Format: YYYYMMDDTHHMMSS, observation start UTC time) passed over the Sundhnúkur volcano area, only orbit 20240823T125304 is presented because most of its pixels over the Sundhnúkur volcano region were near the nadir of the orbit where the data quality is higher. Compared with OMS orbit 20240823\_1036, OMS orbit 20240823\_1217 has a local overpass time closer to that of TROPOMI orbit 20240823T125304 in the volcanic region, making the SO<sub>2</sub> results of OMS orbit 20240823\_1217 more consistent with those of TROPOMI orbit 20240823T125304.

As shown in Fig. 10, both OMS and TROPOMI successfully captured the high SO<sub>2</sub> distribution around the Sundhnúkur volcano on August 23, 2024. The spatial distributions of OMS, TROPOMI DOAS and TROPOMI COBRA SO<sub>2</sub> over Sundhnúkur volcano are similar, but differ at the edge of the SO<sub>2</sub> plume. The correlation between OMS and TROPOMI DOAS reaches ~0.78 over the Sundhnúkur volcano on August 23, 2024, while the correlation between OMS and TROPOMI COBRA reaches ~0.70. However, when SO<sub>2</sub> values exceed 50 DU, OMS SO<sub>2</sub> retrievals are significantly lower than those of TROPOMI DOAS over the Sundhnúkur volcano region on August 23, 2024. Moreover, the relative biases between OMS and TROPOMI DOAS increase with increasing SO<sub>2</sub> columns. This may be attributed to the reason that the OMS SO<sub>2</sub> retrieval uses the 312–326 nm fitting window, where SO<sub>2</sub> has strong absorption and is prone to saturation in the case of high SO<sub>2</sub> concentrations, leading to an underestimation of SO<sub>2</sub> columns. In order to mitigate the risk of saturation, TROPOMI DOAS uses two additional fitting windows (325–335 nm and 360–390 nm) (S5P-BIRA-L2-ATBD-400E) for volcanic eruption cases. In addition, the different overpass time of OMS and TROPOMI, along with varying volcanic eruption

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1160 strength and meteorological conditions, may also be major contributors to the differences in SO<sub>2</sub> columns of OMS and TROPOMI DOAS. The TROPOMI COBRA SO<sub>2</sub> results retrieved from the 310.5–326 nm window are also lower than those from TROPOMI DOAS, but are more consistent with those from OMS.

1165 The Nyamuragira volcano (Region 4 in Fig. 5) is the second case study for comparing FY-3F/OMS SO<sub>2</sub> with TROPOMI DOAS and TROPOMI COBRA 7km SO<sub>2</sub> results over a volcanic eruption. Nyamuragira is Africa's most active volcano and a high-potassium basaltic shield volcano located in the eastern part of the Democratic Republic of the Congo, approximately 25 km north of Lake Kivu and 13 km north-northwest of the Nyiragongo volcano (<https://volcano.si.edu/>). Based on the Volcanic Explosivity Index (VEI) classification (Newhall and Self, 1982) and eruptive history reports of Nyamuragira from the Global Volcanism Program (GVP), the magnitude of Nyamuragira's eruptions can generally be classified as small to moderate. According to the GVP weekly reports, Nyamuragira had continuing eruptive activities in November 2024. The spatial distribution maps (Fig. 11) show that OMS, TROPOMI DOAS, and TROPOMI COBRA results clearly detected the high-concentration SO<sub>2</sub> plume from the Nyamuragira eruption, although the shape of the SO<sub>2</sub> plume differs due to differences in overpass time, observation angles and retrieval strategies. Compared with OMS and TROPOMI DOAS, TROPOMI COBRA shows lower SO<sub>2</sub> columns over the Nyamuragira volcano. Although OMS and TROPOMI DOAS exhibit more comparable SO<sub>2</sub> levels, the quantitative agreement between them is weaker in scatter plot comparisons (not shown). This is primarily because Nyamuragira volcano is located near the equator, unlike the high-latitude Sundhnúkur volcano, making it difficult to identify OMS and TROPOMI orbits with closely matched observation times. Differences in overpass times lead to shifts in plume position, which hampers direct pixel-to-pixel quantitative comparisons over the Nyamuragira region.

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1180 Overall, from the above comparisons between FY-3F/OMS SO<sub>2</sub> and TROPOMI DOAS and TROPOMI COBRA 7km SO<sub>2</sub> results, we can see that FY-3F/OMS has the capability to monitor volcanic activities, and with high spatial resolution of 7 km×7 km and a local overpass time different from TROPOMI, FY-3F/OMS can contribute to a more effective satellite SO<sub>2</sub> product for the continuous monitoring of global volcanic activity.

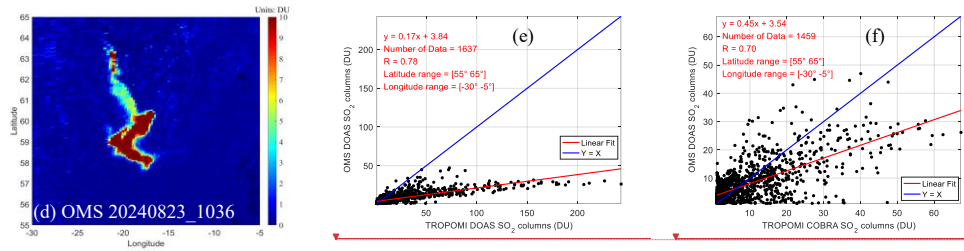
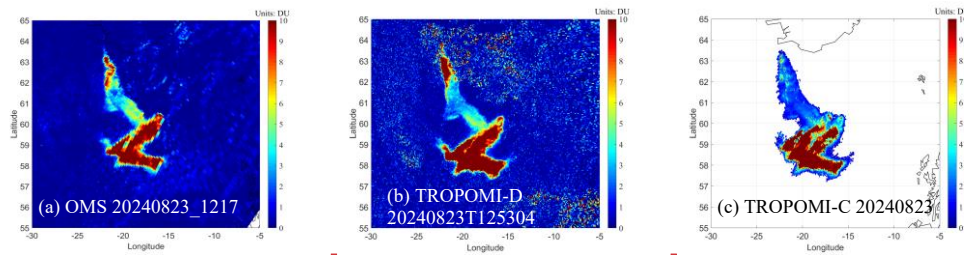
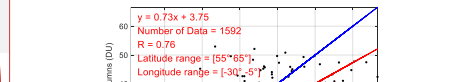
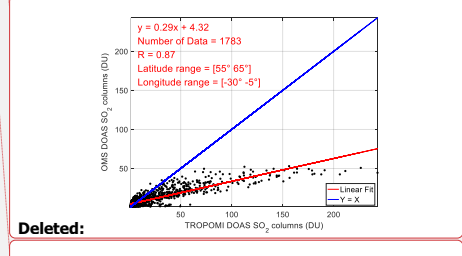
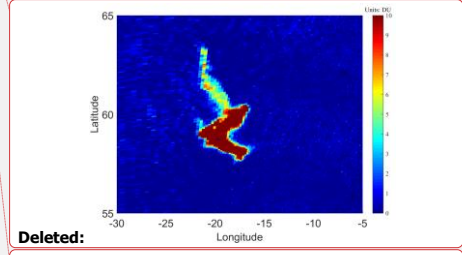
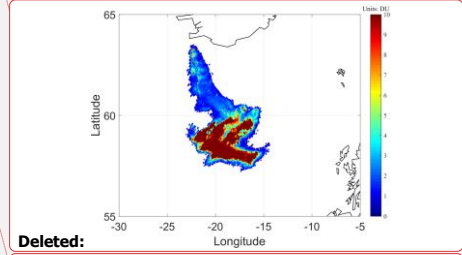
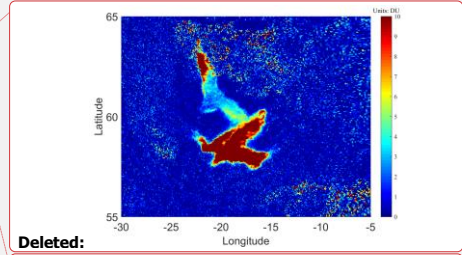
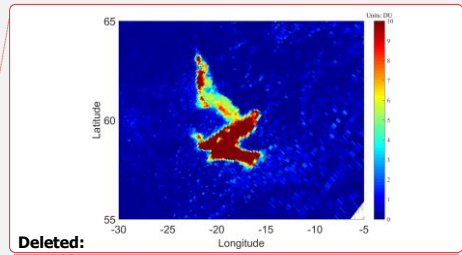


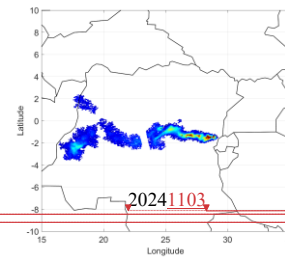
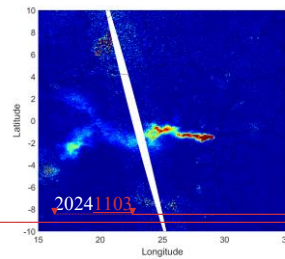
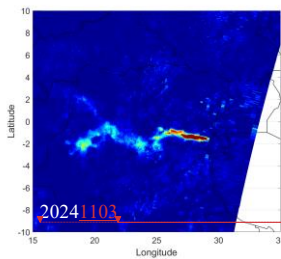
Figure 10: SO<sub>2</sub> retrievals over Sundhnúkur volcano on August 23, 2024. (a, b, c, d) Spatial distribution of **FY-3E/OMS**, **TROPOMI DOAS** and **TROPOMI COBRA 7km SO<sub>2</sub> columns** over Sundhnúkur volcano; (e, f) Scatter plots of **OMS 20240823\_1217** and **TROPOMI** over Sundhnúkur volcano on August 23, 2024, where pixels with SO<sub>2</sub> columns greater than 1 DU were selected and **TROPOMI** is resampled to the latitude-longitude grid of **OMS**. The missing pixels in Figure a are the gap between the two OMS orbits, and the missing pixels in Figure c are **Nan values** due to quality filtering applied to **TROPOMI COBRA** data.

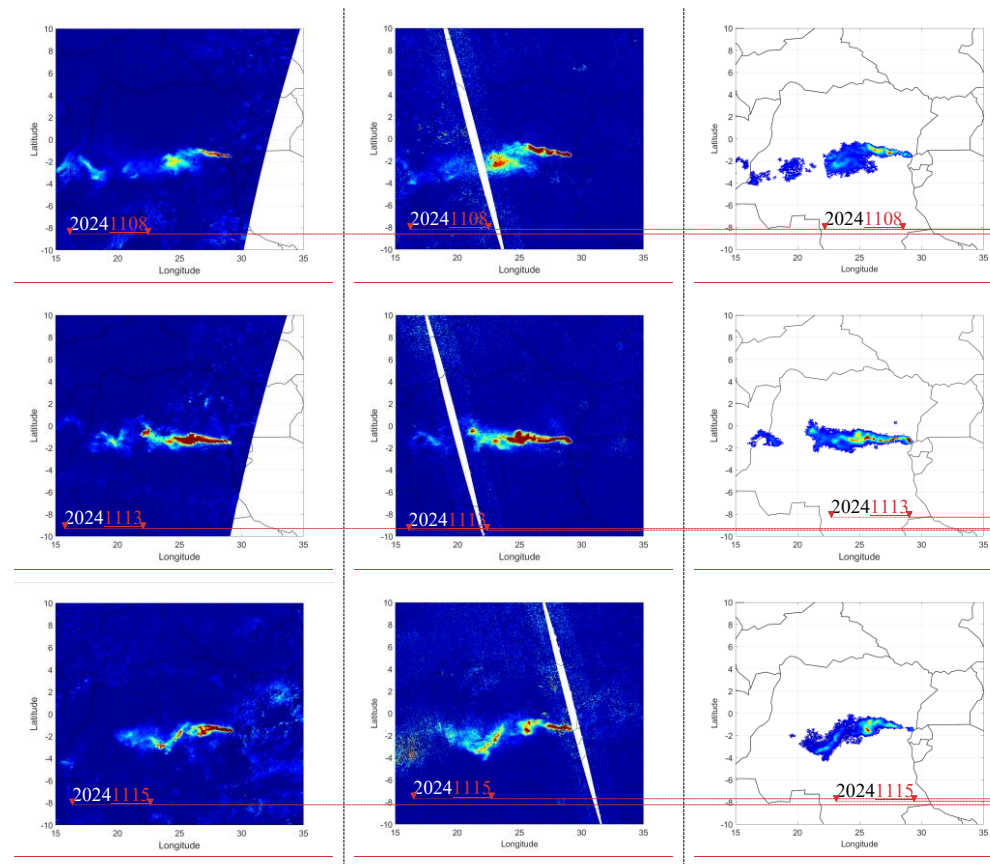


**OMS SO<sub>2</sub> VCDs**

**TROPOMI DOAS SO<sub>2</sub> VCDs**

**TROPOMI COBRA 7km SO<sub>2</sub> VCDs**

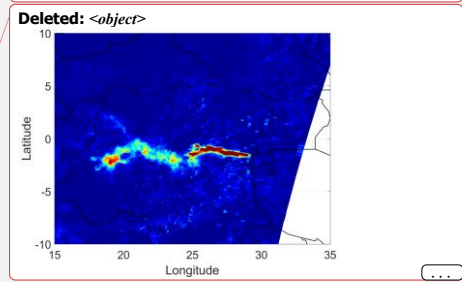




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**Figure 11:** SO<sub>2</sub> retrievals of OMS and TROPOMI over the Nyamuragira volcano on November 3, 8, 13, and 15, 2024. From left to right, the panels show OMS SO<sub>2</sub> VCDs, TROPOMI DOAS SO<sub>2</sub> VCDs, and TROPOMI COBRA 7km L3 SO<sub>2</sub> VCDs. The missing pixels are the gap between the two orbits, or the Nan values due to quality filtering applied to TROPOMI COBRA data.

### 4.3 Comparison ~~over~~ anthropogenic emissions

1300 Compared to the monitoring of high SO<sub>2</sub> emissions from natural sources such as volcanoes, the monitoring of anthropogenic SO<sub>2</sub> emissions from satellite observations is more challenging. ~~The atmospheric SO<sub>2</sub> from anthropogenic emissions is generally much lower compared to that of volcanic eruptions, and is primarily concentrated near the surface. The sensitivity of satellite measurements in the UV band near the surface is relatively low because solar UV radiation is partially absorbed and scattered by atmospheric components such as air, aerosols, and clouds during its transmission. As a result, the weakened UV radiation reaching the boundary layer reduces the sensitivity of satellite instruments to PBL SO<sub>2</sub> and makes it harder to distinguish SO<sub>2</sub> signals from background noise, especially at large solar zenith and satellite viewing angles.~~

1305 Based on the SO<sub>2</sub> emission sources observed by TROPOMI in 2018 (Fioletov et al., 2020), we selected three representative regions – the Persian Gulf (oil and gas exploration, [Region 5 in Fig. 5](#)), Norilsk (smelters, [Region 6 in Fig. 5](#)), and Eastern India (power plants, [Region 7 in Fig. 5](#)) – to compare three SO<sub>2</sub> column products: OMS SO<sub>2</sub>, TROPOMI DOAS SO<sub>2</sub>, and TROPOMI COBRA PBL SO<sub>2</sub>. These comparisons aim at evaluating the capability of OMS in monitoring SO<sub>2</sub> emissions from anthropogenic sources. Similar to the cases of volcanic eruptions, we used all pixels from the TROPOMI DOAS SO<sub>2</sub> product instead of applying QA > 0.5 to filter the high-quality pixels because the QA > 0.5 filter would remove many high SO<sub>2</sub> pixels over anthropogenic emission regions, ~~especially over snow/ice surfaces such as Norilsk. Meanwhile, comparison results for the Persian Gulf and Eastern India regions during the study period show negligible differences whether the QA > 0.5 filter is applied or not (not shown here).~~ In the case of anthropogenic emissions, TROPOMI COBRA L3 grid PBL SO<sub>2</sub> products were used for comparison instead of the COBRA 7km SO<sub>2</sub> products.

1310 The Persian Gulf was selected due to its high anthropogenic emissions, including SO<sub>2</sub> and NO<sub>2</sub>, primarily from oil and gas extraction and refining industries (Mardani et al., 2025; Krotkov et al., 2016). This region has a higher probability of clear-sky days and is located in the low-latitude zone, which means relatively high SNR for satellite observations. As shown in Fig. 12, OMS effectively detects high SO<sub>2</sub> values over the Persian Gulf while maintaining a lower background noise. ~~The variability of enhanced SO<sub>2</sub> columns from OMS are generally consistent with those from TROPOMI DOAS and TROPOMI COBRA. Differences are mainly manifested in magnitude and local-scale variability, which may be attributed to differences in satellite overpass time, retrieval algorithms, AMF, and spatial resolution. Based on the spatiotemporal distributions shown in Fig. 12, three representative days with relatively large and small differences (August 23 and November 4 and 8, 2024) were selected for scatter plot comparisons among the three datasets (OMS SO<sub>2</sub>, TROPOMI DOAS SO<sub>2</sub>, and TROPOMI COBRA PBL SO<sub>2</sub>). Scatter plots (Fig. 13) comparing OMS SO<sub>2</sub> with TROPOMI DOAS and TROPOMI COBRA SO<sub>2</sub> over the Persian Gulf show that: (1) Both TROPOMI DOAS and TROPOMI COBRA SO<sub>2</sub> products exhibit clear positive correlations with OMS, with correlation coefficients (R) ranging from ~0.63 to 0.91. (2) The level of agreement among the three datasets varies with time. On November 4 and 8, OMS shows good consistency with both TROPOMI products, with regression slopes close to unity (DOAS: slopes ≈ 1.00 and 0.98, R = 0.82 and 0.91; COBRA: slopes ≈ 0.93 and 0.96, R = 0.82 and 0.83), indicating good agreement under anthropogenic SO<sub>2</sub> conditions. However, on August 23, OMS retrieves~~

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higher SO<sub>2</sub> columns over the Persian Gulf emission hotspot region than both TROPOMI DOAS and COBRA, with regression slopes of ~1.61 and 2.14, respectively. This discrepancy may be primarily attributed to the relatively low AMFs calculated using GEOS-CF profiles and OMI surface reflectance climatology over these high-SO<sub>2</sub> regions. As shown in Fig. 14, although the corresponding OMS SCD results on August 23 is relatively low, the low AMFs over region with high SCDs lead to enhanced VCD (VCD=SCD/AMF), resulting in higher OMS SO<sub>2</sub> VCDs over these high-SO<sub>2</sub> regions on August 23. (3) For pixels with low SO<sub>2</sub> columns, the correlations among the three datasets are relatively weak, likely due to larger retrieval uncertainties associated with random noise and reduced sensitivity at low SO<sub>2</sub> conditions. It should be noted that Fig. 13 does not present results for consecutive days. This is mainly due to the unavailability of GEOS-CF data for some days, the presence of a large number of pixels located near the satellite swath edges, and/or extensive cloud coverage indicated by the Terra/MODIS true color images, which limit the reliability of the comparison among the three SO<sub>2</sub> datasets. Similar limitations also exist in the India case studies presented later.

Norilsk in northern Russia, located within the Arctic Circle, is one of the world's biggest sources of anthropogenic SO<sub>2</sub> emissions due to its massive nickel and metal smelting industry (Bauduin et al., 2014). With winter lasting 6 to 9 months and snow covering the ground for most of the year, the region's low temperatures and atmospheric stability hinder pollutant dispersion, leading to persistently high SO<sub>2</sub> concentrations over Norilsk. Large SO<sub>2</sub> emissions cause severe air pollution and acid rain, which make Norilsk one of the most polluted cities in the world. On May 16, 2024, the orbits of OMS and TROPOMI with close local overpass times over Norilsk were selected to minimize the influence of emission variability, and meteorological differences on the comparisons of SO<sub>2</sub> columns. As shown in Fig. 15, both OMS and TROPOMI were able to detect the high SO<sub>2</sub> plumes over the Norilsk region, with similar spatial patterns and transport features. The SO<sub>2</sub> columns from OMS and TROPOMI DOAS show strong correlations, with correlation coefficients ranging from 0.80 to 0.85 over the Norilsk region. However, OMS SO<sub>2</sub> VCD retrievals are lower than those from TROPOMI DOAS, with the average relative biases ( $(|OMS - TROPOMI|) / TROPOMI$ ) of the data from the Norilsk region in OMS orbit 20240516\_0334 being approximately 38% (excluding SO<sub>2</sub> columns smaller than 1 DU), and for OMS orbit 20240516\_0516 being approximately 33% (applying the same filtering criteria). These differences may be related to differences in AMF strategy, retrieval algorithm, and spatial resolution. In contrast, the TROPOMI COBRA PBL L3 products exhibits large data gaps due to quality filtering over the Norilsk region, limiting its applicability over Norilsk for this case. In addition, the Terra/MODIS true color image from the same day shows the presence of snow cover over the Norilsk region, highlighting OMS's capability to capture anthropogenic SO<sub>2</sub> emissions in high-latitude regions within the Arctic Circle.

India's SO<sub>2</sub> emissions are mainly from coal fired power plants, transportation, and agricultural activities, which are growing rapidly, increasing by more than 100% from 2005 to 2015 (Krotkov et al., 2016; Kuttippurath et al., 2022). Eastern India, in particular, is a major hotspot due to the dense distribution of coal-based power plants and industrial facilities. As shown in Fig. 16, OMS successfully captured strong SO<sub>2</sub> plumes over Eastern India on 4, 5, 8, and 9 November 2024, with spatial patterns that are generally consistent with those retrieved by TROPOMI DOAS and TROPOMI COBRA. Figure 16 also includes Terra/MODIS true color images for the same days, which indicate relatively low cloud coverage over Eastern India.

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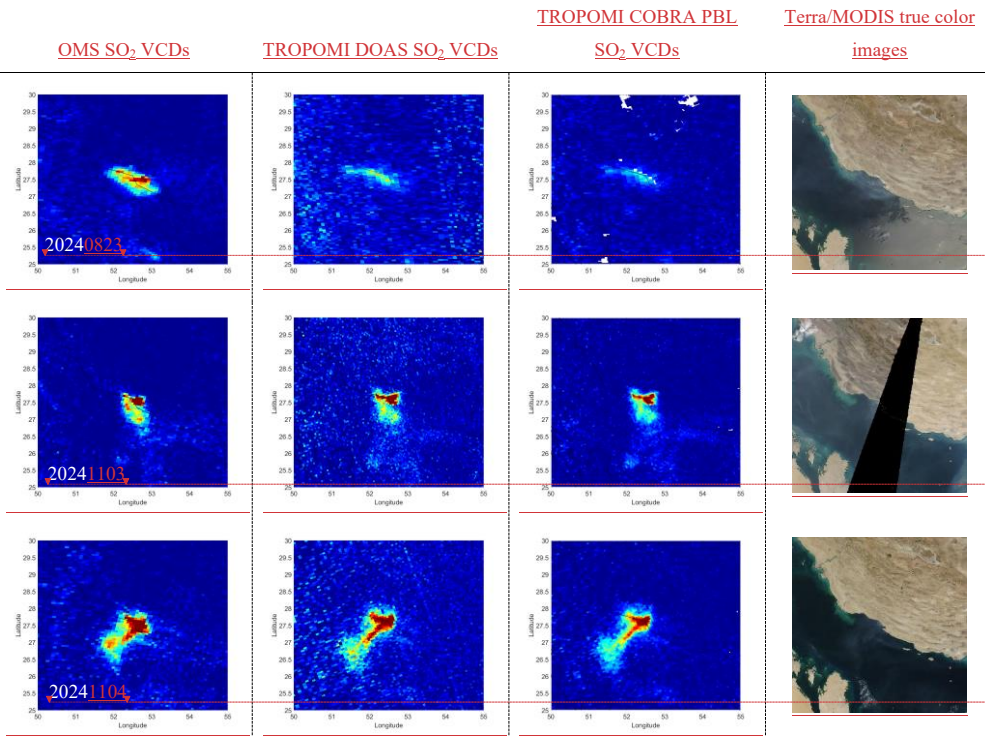
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thereby minimizing the influence of clouds on the intercomparison of SO<sub>2</sub> retrievals. Despite the overall consistency in spatial distribution, OMS SO<sub>2</sub> retrievals over regions with strong SO<sub>2</sub> emissions are higher than those from TROPOMI DOAS and TROPOMI COBRA on November 5, 8, and 9, 2024. This overestimation is likely related to uncertainties in AMF calculations associated with the use of GEOS-CF SO<sub>2</sub> vertical profiles, OMI surface reflectance climatology, and aerosol loading over Eastern India. To further improve the accuracy of OMS SO<sub>2</sub> retrievals over India, future work will focus on incorporating more representative local SO<sub>2</sub> vertical profiles and more accurate surface reflectance databases. Overall, the comparisons over the Persian Gulf, Norilsk, and Eastern India demonstrate that OMS SO<sub>2</sub> retrievals show good spatial consistency and strong correlations with TROPOMI DOAS and TROPOMI COBRA SO<sub>2</sub> products; OMS is capable of effectively distinguishing intense anthropogenic SO<sub>2</sub> signals from background noises. Owing to differences in local overpass times, OMS can provide effective complementary data to fill the monitoring gaps in TROPOMI SO<sub>2</sub> products.



**Moved down [1]:** Figure 18 also shows that due to different local overpass times, when the SO<sub>2</sub> pollution area in India is located at the edge of the TROPOMI orbit where large retrieval errors often occur, OMS can provide effective data support to fill the monitoring gaps caused by TROPOMI's edge-related pixels. These comparisons

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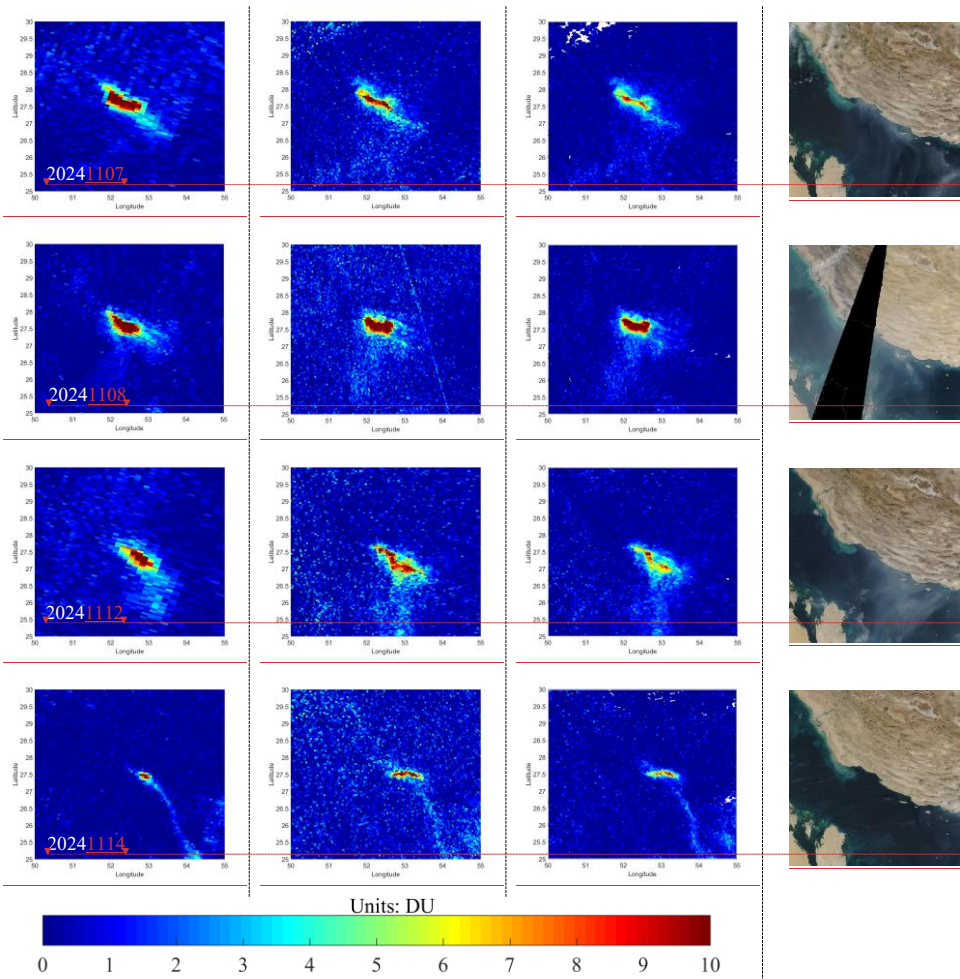
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**Figure 12: SO<sub>2</sub> retrievals of OMS and TROPOMI over the Persian Gulf on August 23, 2024, and November 3, 4, 7, 8, 12, and 14, 2024. From left to right, the panels show OMS SO<sub>2</sub> VCDs, TROPOMI DOAS SO<sub>2</sub>, TROPOMI COBRA PBL L3 SO<sub>2</sub>, and Terra/MODIS true color images. Each row corresponds to the same observation date. The missing pixels are Nan values due to quality filtering applied to TROPOMI COBRA data.**

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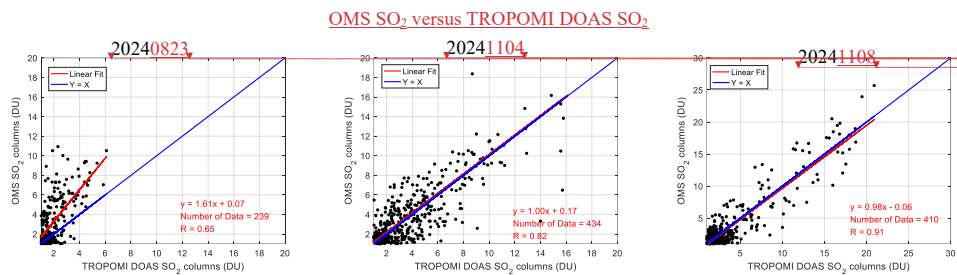
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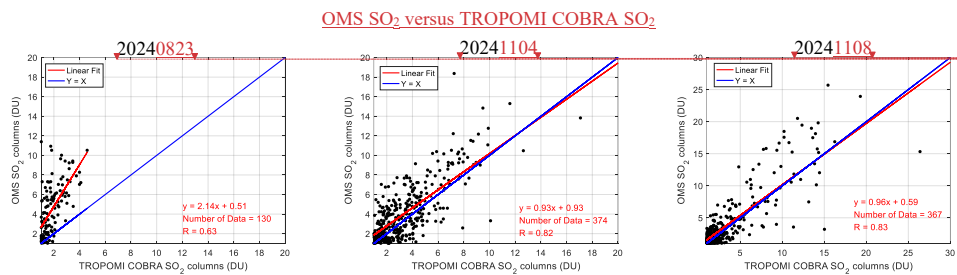
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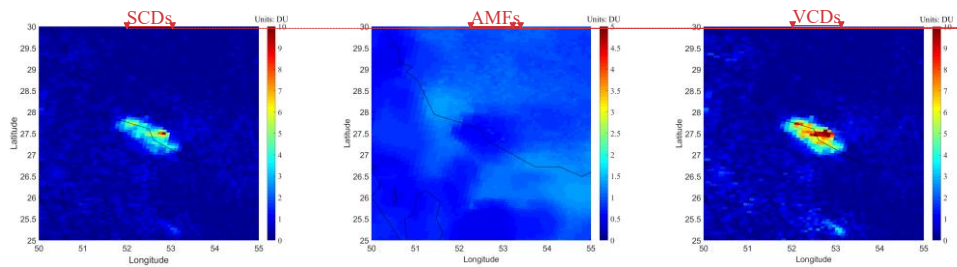
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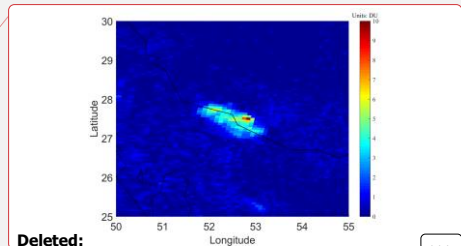


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**Figure 13: Scatter plots of FY-3F/OMS, TROPOMI DOAS and TROPOMI COBRA PBL SO<sub>2</sub> over the Persian Gulf on August 23 and November 4 and 8, 2024. Pixels with SO<sub>2</sub> columns greater than 1 DU were selected, and TROPOMI data were resampled to the latitude-longitude grid of OMS. Data points in the scatter plots were selected from latitude 25°–30° N and longitude 50°–55° E.**



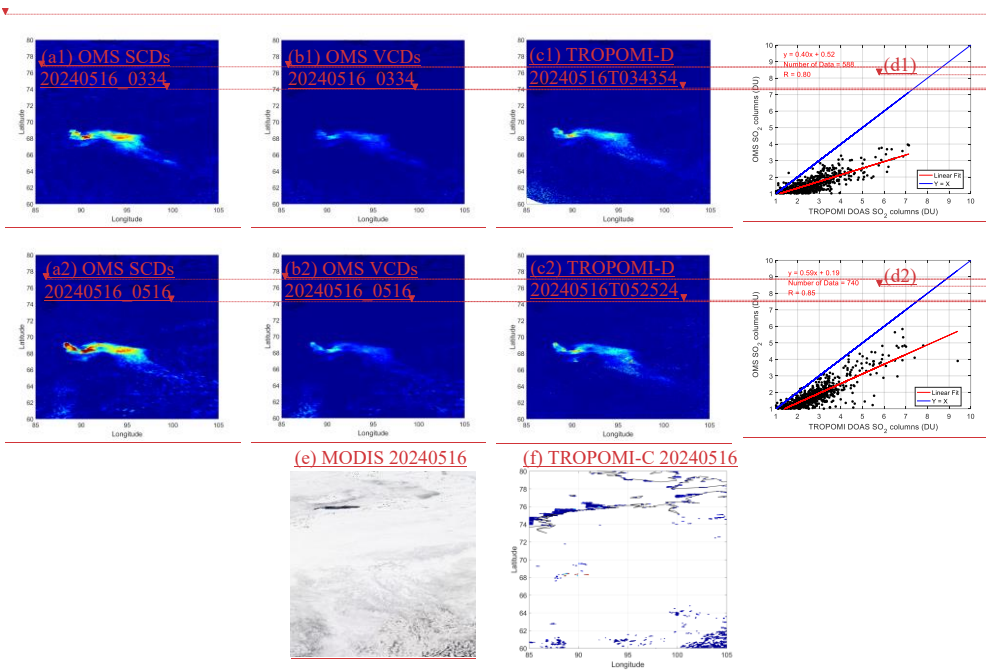
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**Figure 14: Spatial distribution of FY-3F/OMS SO<sub>2</sub> SCDs, AMFs, and VCDs over the Persian Gulf on August 23, 2024.**

VCDs=SCDs/AMFs.



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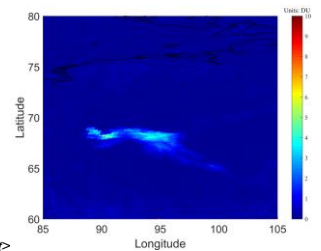
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**Figure 15: SO<sub>2</sub> retrievals over Norilsk on May 16, 2024. (a1-2, b1-2, c1-2) Spatial distribution of FY-3F/OMS and TROPOMI DOAS SO<sub>2</sub> columns over Norilsk; (d1-2) Scatter plots of OMS and TROPOMI DOAS SO<sub>2</sub> columns over Norilsk on May 16, 2024, where pixels with SO<sub>2</sub> columns greater than 1 DU were selected within 60–80°N and 85–105°E, and TROPOMI were resampled to the latitude-longitude grid of OMS; (e) True Color Image of Norilsk from Terra/MODIS on May 16, 2024; (f) SO<sub>2</sub> columns from TROPOMI COBRA PBL over Norilsk on May 16, 2024. Note that the missing pixels in Figure f are due to quality filtering applied to TROPOMI COBRA data.**

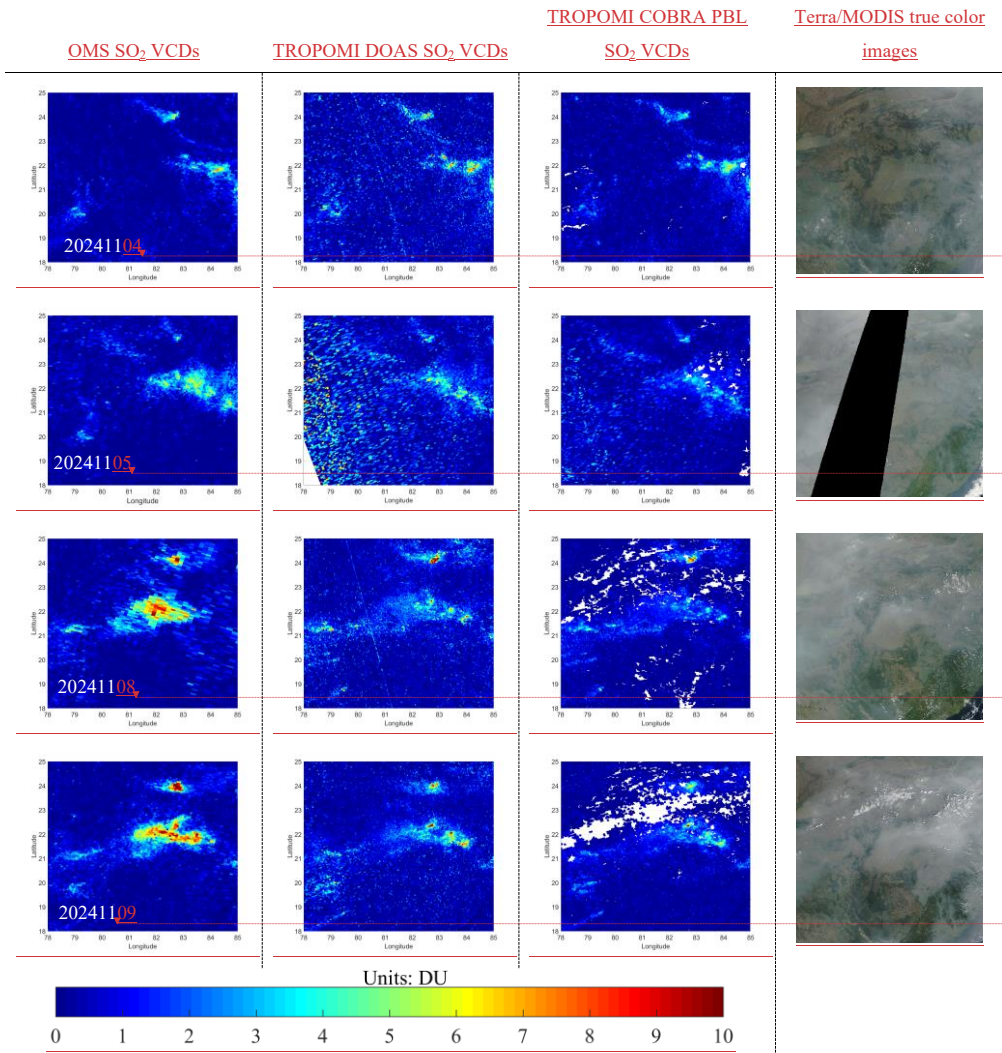
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**Figure 16:** SO<sub>2</sub> retrievals of OMS and TROPOMI over Eastern India on November 4, 5, 8, and 9, 2024. From left to right, the panels show OMS SO<sub>2</sub> VCDs, TROPOMI DOAS SO<sub>2</sub>, TROPOMI COBRA PBL L3 SO<sub>2</sub>, and Terra/MODIS true color images.

Each row corresponds to the same observation date. The missing pixels are the gap between the two orbits, or the Nan values due to quality filtering applied to TROPOMI COBRA data.

## 5 Error analysis

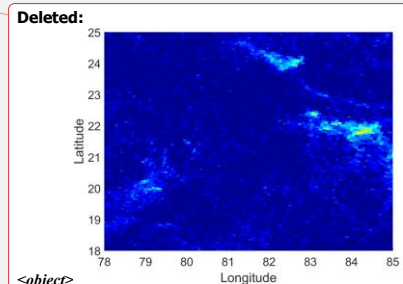
The main error sources in the OMS DOAS SO<sub>2</sub> retrieval include instrument-related errors, DOAS SCD spectral fitting errors, AMF uncertainties, and the residual error after background offset correction (see also, e.g., Lee et al., 2009; Theys et al., 2017). Instrument-related errors include spectral and radiometric calibration errors, degradation of the instrument, stray light contamination and non-uniformity of the diffuser plate, which introduce systematic biases in both radiance and irradiance measurements. DOAS SCD spectral fitting errors include uncertainties in the absorption cross-sections of SO<sub>2</sub> and O<sub>3</sub>, interference from strong O<sub>3</sub> absorption, the Ring effect caused by inelastic scattering, and the selection of the polynomial order in spectral fitting. The AMF, which is crucial for the accuracy of OMS SO<sub>2</sub> retrieval, is mainly affected by the uncertainties in surface reflectance, SO<sub>2</sub> vertical profile shape, wavelength dependence, and terrain height. Moreover, the background offset correction may introduce additional uncertainties, especially in high SO<sub>2</sub> areas.

This section is organized as follows. First, the major error sources affecting the SCD retrieval are listed, and the quantitative uncertainty of the OMS SO<sub>2</sub> SCD retrieval is provided. Second, the main error sources influencing the AMF are analysed, and the AMF uncertainty associated with each error component is quantitatively estimated. Third, the residual errors after background offset correction are evaluated. Finally, based on the above results, overall quantitative estimates of the uncertainty of OMS SO<sub>2</sub> retrieval are presented.

### 5.1 Errors in SCD

**Table 4. Main error sources affecting the OMS SO<sub>2</sub> SCD retrieval**

Parameter	Parameter uncertainty or resulting SCD uncertainty
<u>OMS-N L1 absolute radiometric calibration error (requirements)</u>	<3%
<u>OMS-N L1 relative radiometric calibration error (requirements)</u>	<2%
<u>OMS-N L1 spectral calibration error (requirements)</u>	~0.01nm
<u>OMS-N L1 diffuser calibration accuracy (requirements)</u>	<3%
<u>OMS-N L1 noise requirements</u>	Signal-to-noise ratio > 250 in the wavelength range 312–340 nm
<u>TSIS-1 HSRS reference spectrum uncertainty</u>	~0.3%
<u>Absorption cross-section uncertainty</u>	~3%
<u>Use of a fixed Ring spectrum</u>	SCD uncertainty < 3.5%



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Considering these error sources and assuming that they are independent of each other, the total uncertainty in the retrieved SO<sub>2</sub> column can be approximated as:

$$\sigma_{SO_2} = \sqrt{\left(\frac{\sigma_{SCD}}{AMF}\right)^2 + \left(\frac{\sigma_{SCD}^{back}}{AMF}\right)^2 + \left(\frac{(SCD-SCD^{back})\sigma_{AMF}}{AMF^2}\right)^2}$$

(Eq. 3)

where  $\sigma_{SCD}$  is the random error from DOAS SO<sub>2</sub> SCD spectral fitting including instrument-related noise,  $\sigma_{SCD}^{back}$  is the residual systematic error after background offset correction, and  $\sigma_{AMF}$  is the AMF uncertainty which includes two components: one is related to the atmospheric scattering weight and the other one is associated with the SO<sub>2</sub> profile shape.

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Retrieval fitting window and low-order polynomial                      SCD uncertainty < 11%  
 Others (e.g., stray light, dark current, ISRF, interference from strong O<sub>3</sub> absorption in the fitting window)                      =

The main error sources affecting OMS SO<sub>2</sub> SCD primarily include instrument-related noise and algorithm settings in spectral fitting (Table 4). These error sources are difficult to separate, making it challenging to quantitatively estimate how each individual error source contributes to the SCD retrieval uncertainty. Although OMS L1 provides specified performance requirements before launch, on-orbit measurements indicate that the OMS L1 errors deviate from the planned specifications for certain parameters. At the time of writing, the updated OMS L1 errors have not yet been obtained. Therefore, in this study, we do not report the contribution of each individual error source to the final SCD uncertainty. Instead, we use the DOAS Spectral Fitting Error (SFE) to derive the overall SCD uncertainty under the current OMS L1 instrument status and DOAS settings.

#### 5.1.1 Error source: instrument-related errors

The errors in irradiance and radiance measurements are the main instrument-related error sources affecting OMS SO<sub>2</sub> SCD retrievals, leading to systematic biases such as along-track stripes at specific viewing angles and cross-track asymmetry in SO<sub>2</sub> SCD retrievals (Boersma et al., 2004). To reduce errors related to irradiance non-uniformity, the TSIS-1 HRSR hybrid solar reference spectrum was used instead of the OMS irradiance measurements to mitigate the effects of viewing angle dependence and instrument degradation on OMS SO<sub>2</sub> retrieval. Radiance measurement errors mainly depend on viewing angle, wavelength, and optical degradation. The viewing angle dependence, primarily caused by calibration inaccuracies, results in unequal responses across different cross-track positions. These biases can be partially corrected using background offset correction but cannot be fully eliminated. With increasing optical degradation over the OMS on-orbit lifetime, additional errors may be introduced into the OMS radiance spectra, thereby leading to larger uncertainties of OMS SO<sub>2</sub> SCD retrievals.

#### 5.1.2 Error source: absorption cross-sections

The temperature dependence and uncertainties of absorption cross-section spectra is one of the error sources which affect the accuracy of OMS SCD retrieval. The OMS SO<sub>2</sub> SCD retrieval utilizes the Bogumil SO<sub>2</sub> and O<sub>3</sub> absorption cross-section spectra at constant 273 K and 223 K (Bogumil et al., 2003), which is in general not representative of the effective temperature corresponding to the SO<sub>2</sub> vertical profile. The differences in SCD retrievals caused by temperature-dependent absorption cross-sections increase with increasing SO<sub>2</sub> columns (Yan et al., 2014). For example, compared to SCD retrievals using the 203 K absorption cross-sections, the differences in SO<sub>2</sub> SCDs can reach a maximum of ~25 DU (with SCDs around 60 DU). In addition to the temperature dependence, the uncertainties of the 273 K SO<sub>2</sub> and 223 K O<sub>3</sub> absorption cross-sections from Bogumil et al. (2003) are approximately 3.0%, which may result in ~6% systematic errors in the retrieved SO<sub>2</sub>

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- Deleted:** The OMS irradiance and radiance uncertainties mainly depend on viewing angle, wavelength, and optical degradation. The viewing angle dependence, caused by calibration inaccuracies, results in unequal responses for all viewing angles (one viewing angle corresponds to one cross-track position). With increasing optical degradation and inaccurate spectral calibration, more errors can be introduced into the irradiance and radiance spectra. This degradation is difficult to monitor and calibrate, because no accurate standards over the full OMS wavelength range are readily available. ...
- Deleted:** Meanwhile, these errors in solar irradiance and earth radiance are not constant and can change with time and location, making it difficult to correct their impact on SO<sub>2</sub> retrievals. After one year in orbit, the intensity of OMS irradiance at the shorter wavelength of 317 nm has decreased by about 8.83%, while at the longer wavelength of 331 nm, it has decreased by about 6.07%. Using the TSIS HRSR hybrid solar reference spectrum instead of the OMS irradiance measurements can mitigate the impact of viewing angle dependence and degradation on OMS SO<sub>2</sub> retrieval. However, since the solar reference spectrum does not contain the instrument characteristics, it may introduce systematic overestimation or underestimation in SO<sub>2</sub> column retrievals. These systematic biases caused by the TSIS HRSR can be partially reduced through background offset correction but cannot be fully eliminated.
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590 [SCD within the 312–326 nm fitting window \(Vandaele et al., 2009\)](#). Future work will incorporate accurate temperature correction in OMS SO<sub>2</sub> retrievals.

### 5.1.3 Error source: Ring effect

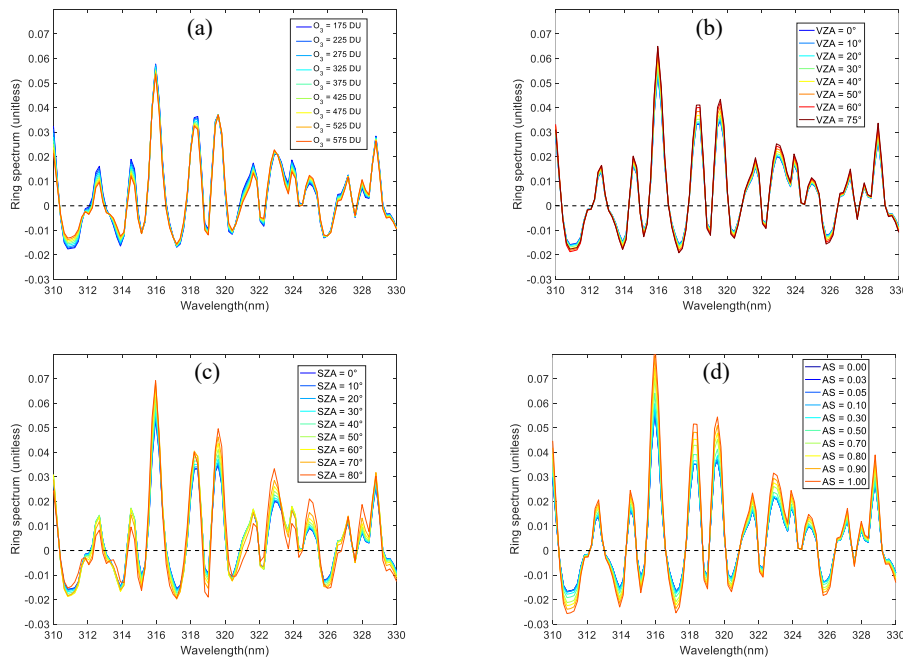


Figure 17: Variation of Ring spectrum with O<sub>3</sub>, VZA, SZA and surface reflectivity (AS). Ring spectrum was calculated using the SCIATRAN model, convolved with the OMS ISRF. The default SCIATRAN settings for the Ring spectrum are as follows: wavelength step=0.2 nm, clear sky, HS=0 km, O<sub>3</sub>=275 DU, AS=0.05, SZA=30°, VZA=0°, RAA=0°.

In the UV wavelength band, the Ring effect is a non-negligible part of the DOAS SCD fitting process. Taking the OMS 20240823\_1036 orbit as an example, after including the Ring spectrum into the DOAS retrieval, the spectral fitting RMSE decreases by approximately 0.004 to 0.01. As shown in Fig. 17, the Ring spectrum varies with SZA, VZA, O<sub>3</sub> 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<sub>3</sub> column varies from 175 DU to 575 DU, 47.34% (absolute deviation: 0.0048) as the AS varies from 0 to 1, 24.18%

**Deleted:** is also one of the error sources in the SO<sub>2</sub> SCD retrievals. Systematic errors in slant columns due to SO<sub>2</sub> cross-section uncertainties are estimated to be around 6% in the 312–326 nm fitting window (Vandaele et al., 2009). The uncertainty of the SO<sub>2</sub> absorption cross-sections from Bogumil et al. (2003) varies with temperature, being 2.8% at 293 K and 3.0% at lower temperatures. The uncertainty of O<sub>3</sub> absorption cross-sections from Bogumil et al. (2003) is approximately 3.1% or less. Therefore, to improve the accuracy of OMS SO<sub>2</sub> retrievals, it is essential to account for the variations in the SO<sub>2</sub> absorption cross-section with temperature and altitude, especially in cases of volcanic eruptions. ...

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**Deleted:** 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<sub>3</sub> 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<sub>3</sub> 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<sub>2</sub> for all pixels. The reason is that although the Ring spectrum varies significantly with SZA, VZA, O<sub>3</sub> column, and AS within the 310–330 nm wavelength range, the impact of Ring spectrum variability on SO<sub>2</sub> 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<sub>2</sub> concentrations. Moreover, using Ring spectra that vary with SZA, VZA, O<sub>3</sub> 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<sub>2</sub> column retrievals.

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Additionally, the accuracy of DOAS SCD fitting is also influenced by the following factors: (1) Interference from strong O<sub>3</sub> absorption in the retrieval fitting window. Due to the overlap of O<sub>3</sub> and SO<sub>2</sub> absorption in the UV wavelength and the fact that the atmospheric O<sub>3</sub> absorption is often much higher than that of SO<sub>2</sub>, the UV radiation reaching the near-surface (the primary altitude of anthropogenic SO<sub>2</sub> emissions) is weakened, resulting in a lower SNR. When using the weakened radiance and DOAS fitting to simultaneously retrieve O<sub>3</sub> and SO<sub>2</sub>, the strong O<sub>3</sub> absorption signal may overshadow the SO<sub>2</sub> absorption information, leading to errors in the DOAS SO<sub>2</sub> SCD retrievals. Sensitivity analysis shows that a 1% increase in O<sub>3</sub> can lead to approximately a 5% decrease in DOAS SO<sub>2</sub> retrievals (Yan et al., 2017). (2) Selection of retrieval fitting window. Different retrieval fitting windows have varying SO<sub>2</sub> absorption features, O<sub>3</sub> absorption interference, and SNR. The scheme using a single retrieval fitting window of 312–326 nm for OMS SO<sub>2</sub> SCD retrieval may lead to the underestimation of SO<sub>2</sub> columns in ...

1690 (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°.

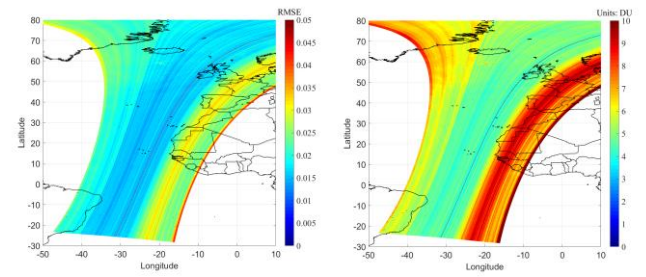
1695 However, in this study, a fixed Ring spectrum calculated from SCIATRAN was used to retrieve SO<sub>2</sub> for all OMS pixels. The reason is that although the Ring spectrum varies significantly with SZA, VZA, O<sub>3</sub> column, and AS within the 310–330 nm wavelength range, the impact of Ring spectrum variability on SO<sub>2</sub> retrievals is relatively small (<3% or less) due to the weak correlation between the Ring spectrum and the satellite TOA reflectance, especially in the case of volcanic eruptions with high SO<sub>2</sub> concentrations. Moreover, using Ring spectra that vary with SZA, VZA, O<sub>3</sub> 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<sub>2</sub> column retrievals.

#### 5.1.4 Error source: others

1700 The OMS SO<sub>2</sub> SCD retrieval is also influenced by the following factors: (1) Interference from strong O<sub>3</sub> absorption in the retrieval fitting window. Due to the overlap of O<sub>3</sub> and SO<sub>2</sub> absorption in the UV wavelength, the strong O<sub>3</sub> absorption signal may overshadow the SO<sub>2</sub> absorption information, leading to errors in SO<sub>2</sub> SCD retrievals. (2) Selection of fitting window. Different retrieval fitting windows have varying SO<sub>2</sub> absorption features, O<sub>3</sub> absorption interference, and SNR. The scheme using a single retrieval fitting window of 312–326 nm for OMS SO<sub>2</sub> SCD retrieval may lead to the underestimation of SO<sub>2</sub> columns in the cases of volcanic eruptions. (3) Low-order polynomial. In DOAS retrievals, low-order polynomials are used to remove slow-varying components, such as aerosol scattering and broad spectral features of absorption. In this study, a third-order polynomial was used for SCD spectral fitting. The errors introduced by this polynomial will need to be quantified.

#### 5.1.5 Total SCD uncertainties

1710 Taking a volcanic eruption orbit as an example (wide range of measured SCDs; orbit OMS 20240823\_1036), two plots of the SCD fitting RMSE and SFE are presented. As shown in Fig. 18, both RMSE and SCD uncertainty are relatively large and exhibit pronounced striping patterns. At the right edge of the swath, the SCD uncertainty exceeds 8 DU, while at the left edge it is approximately 5–6 DU. In the middle of the swath, the SCD uncertainty is about 3–5 DU. These large SCD uncertainties are mainly associated with instrument radiometric and spectral calibration errors. Although background offset corrections can substantially reduce striping patterns in the SO<sub>2</sub> columns, separating the contributions of instrument-related noise and spectral fitting errors to the overall SCD uncertainty remains challenging. Ongoing improvements to the OMS L1 data are expected to reduce striping and calibration asymmetries, thereby improving the accuracy of SO<sub>2</sub> SCD retrievals.



**Figure 18: RMSE and SFE of OMS SO<sub>2</sub> SCDs for OMS orbit 20240823 1036.**

## 5.2 Errors in AMF

AMF uncertainty is a primary source of the uncertainty of OMS SO<sub>2</sub> VCD retrieval. In this study, OMS SO<sub>2</sub> AMFs were calculated using SO<sub>2</sub> vertical profiles from GEOS-CF (Keller et al., 2021) and Box-AMFs derived from the SCIATRAN model (Chen et al., 2009; Wagner et al., 2007; Palmer et al., 2001; Boersma et al., 2004; see Section 3.4 for more information). The uncertainty in OMS SO<sub>2</sub> AMF is mainly associated with SZA, VZA, RAA, AS, HS, O<sub>3</sub> column, the shape of SO<sub>2</sub> vertical profile ( $S(z)$ ), and wavelength ( $\lambda$ ) dependence (Lee et al., 2009). It should be noted that the clouds and aerosols were not considered in the OMS SO<sub>2</sub> AMF calculation. Therefore, AMF uncertainties associated with clouds and aerosols were not included in the present AMF error analysis.

In this section, sensitivity tests of OMS SO<sub>2</sub> AMF were conducted using the SCIATRAN model by computing Box-AMFs under different forward-model configurations (Fig. 19). And then the contribution of each input parameter to the AMF uncertainty was quantified by perturbing it according to its estimated uncertainty while keeping other parameters fixed.

Finally, an overall estimate of uncertainty in OMS SO<sub>2</sub> AMF was derived. For the perturbation analysis, a set of typical atmospheric and surface conditions was adopted as the default configuration, with SZA=32.9°, VZA=0°, RAA=0°, AS=0.05, HS=0 km, wavelength=320 nm, O<sub>3</sub> column=275 DU, clear-sky conditions, and with the assumption of surface reflectance as isotropic Lambertian equivalent reflector (LER).

The contributions of different parameters to the AMF uncertainty were evaluated across five scenarios: clean, boundary-layer pollution, boundary-layer pollution over snow and ice, volcanic degassing, and volcanic eruption. To represent these scenarios, four assumed SO<sub>2</sub> vertical profiles were constructed (Fig. 20), corresponding to clean conditions (SO<sub>2</sub> column=0.11 DU), anthropogenic SO<sub>2</sub> emissions (SO<sub>2</sub> column=5 DU), volcanic degassing with plume heights around 2 km (SO<sub>2</sub> column=16.5 DU), and volcanic eruptions with plume heights around 6 km (SO<sub>2</sub> column=120 DU).

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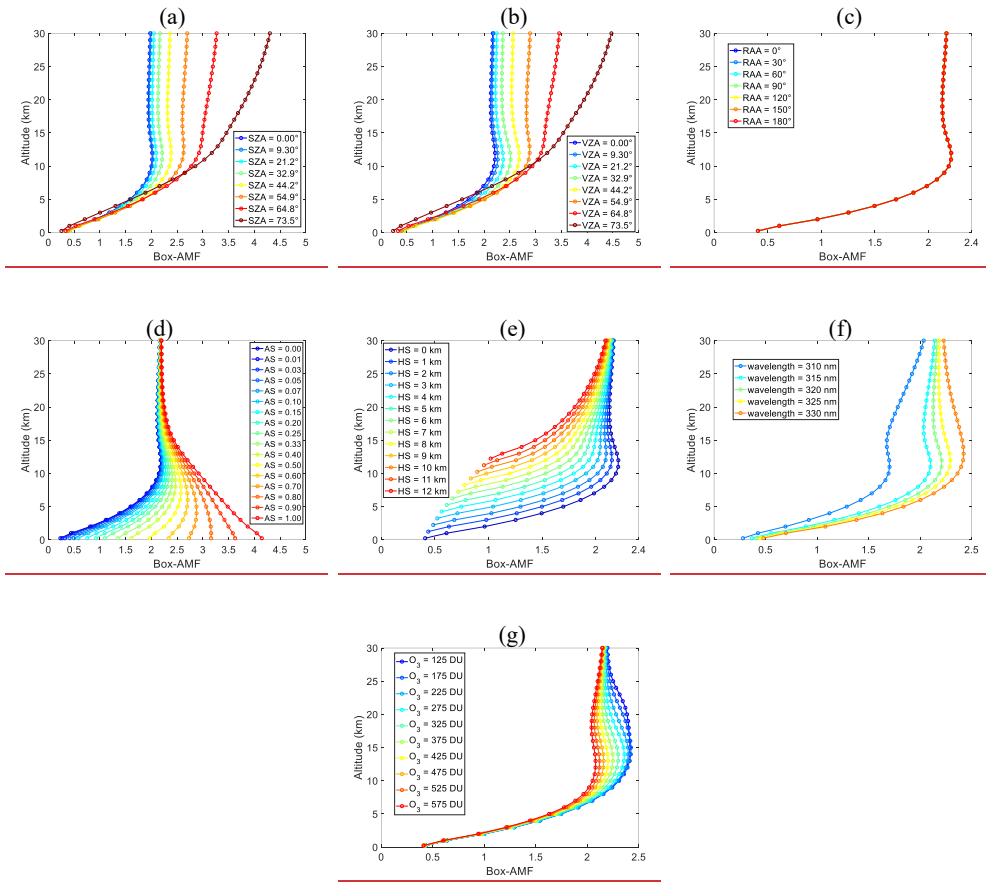
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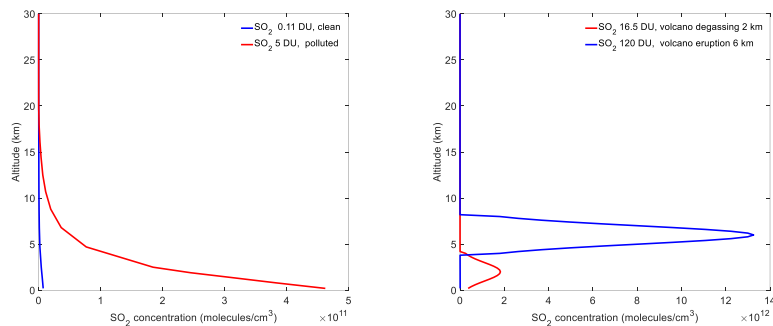
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**Figure 19: Variation of Box-AMF with SZA, VZA, RAA, AS, HS, wavelength, and O<sub>3</sub> column. The default SCIATRAN settings for Box-AMF calculation are as follows: wavelength=320 nm, clear sky, HS=0 km, O<sub>3</sub>=275 DU, AS=0.05, SZA=32.9°, VZA=0°, RAA=0°.**



**Figure 20: (Left) Assumed SO<sub>2</sub> profiles corresponding to clean conditions, and anthropogenic SO<sub>2</sub> emissions; (Right) Assumed SO<sub>2</sub> profiles corresponding to volcanic degassing with plume heights around 2 km, and volcanic eruption with plume heights around 6 km.**

### 5.2.1 Error source: observation angles (SZA, VZA, RAA)

As shown in Figs. 19a-b, at lower altitudes, Box-AMF is relatively insensitive to changes in SZA and VZA within the range of 0–50°. However, at higher altitudes (e.g., above 5km), the Box-AMF generally increases with increasing SZA and VZA due to the longer atmospheric path length at larger angles, which enhances the contribution of each atmospheric layer to the total AMF. When SZA or VZA exceeds 73.5°, Box-AMFs decrease significantly, below altitude 10 km, and larger angles are excluded. As shown in Fig. 19c, the variation of Box-AMF with RAA is negligible. At the time of writing, the measurement errors of OMS SZA and VZA are unavailable, and the proportion of uncertainty propagated to the AMF remains to be determined. In general, satellite measurements of SZA and VZA are considered highly accurate, and their contribution to the overall uncertainty is expected to be negligible.

### 5.2.2 Error source: surface reflectance (AS)

The surface reflectance has a relatively strong impact on the OMS SO<sub>2</sub> AMF values, especially in anthropogenic emission regions where SO<sub>2</sub> is concentrated near the surface. As shown in Fig. 19d, Box-AMF increases with increasing surface reflectance due to enhanced atmospheric multiple scattering. The difference in surface Box-AMF can reach approximately 1700%.

The OMI surface LER database used for OMS SO<sub>2</sub> AMF calculation has overall uncertainties in the LER of 0.01–0.02, with slightly increasing values at shorter wavelengths (Kleipool et al., 2008). Here, we assume an LER uncertainty of 0.02 and use the SO<sub>2</sub> vertical profiles shown in Fig. 20 to calculate the AMF uncertainty due to AS errors for five scenarios. The results are as follows: (1) AMF uncertainty decreases with increasing AS, indicating that bright surfaces reduce the effect of

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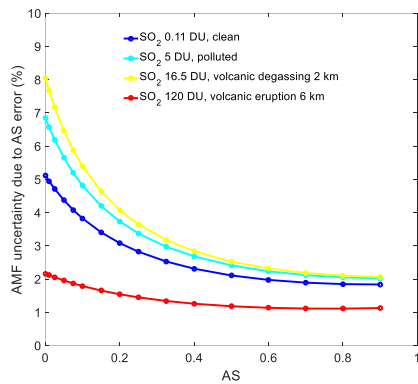
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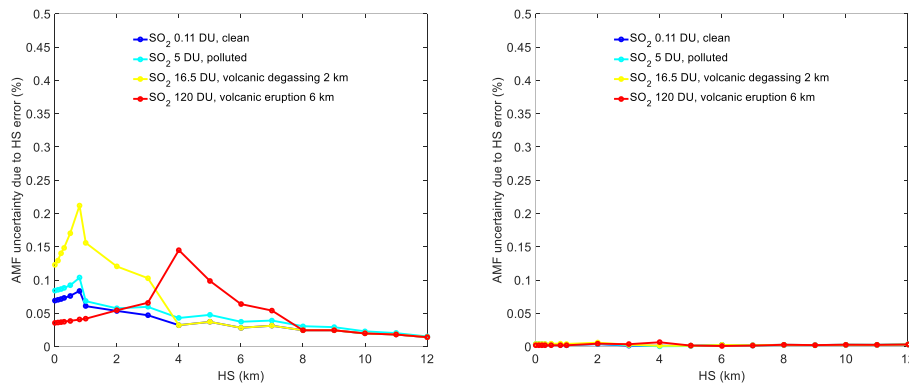
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805 AS perturbations on AMF. (2) Volcanic degassing and polluted conditions are particularly sensitive to AS: at AS = 0.05, uncertainties are ~6.5% and ~5.6%, respectively, while at AS = 0.8, they decrease to ~2.1% and ~2.0%, indicating that AS strongly influences AMF in cases with moderate SO<sub>2</sub> concentrations. (3) High-concentration SO<sub>2</sub> is less sensitive to AS: for volcanic eruption scenarios, AMF uncertainty varies slightly with AS, ranging from 1.1% to 2.1%. These results indicate that accurate AS input is crucial for reliable AMF calculations. In the future, higher spatial resolution surface reflectance  
810 products that account for directional effects, such as the TROPOMI DLER model (Tilstra et al., 2024), will be considered for OMS SO<sub>2</sub> AMF calculations.



**Figure 21:** AMF uncertainty due to AS errors for different scenarios.

### 5.2.3 Error source: terrain height (HS)



**Figure 22:** AMF uncertainty due to HS errors for different scenarios. (Left) AS=0.05; (Right) AS=0.8.

The terrain heights used in OMS SO<sub>2</sub> AMF calculations were obtained from the OMS L1 dataset, which derived terrain information from the Copernicus Digital Elevation Model (COP-DEM) with a spatial resolution of 30 m. According to the Copernicus DEM Product Handbook, the product exhibits an absolute vertical accuracy better than 4 m and a horizontal accuracy better than 6 m under standard conditions (Fahrland et al., 2020). Therefore, a terrain height uncertainty of 4 m is assumed to quantify the AMF uncertainty induced by HS errors.

The results (Fig. 22) show that: (1) For AS = 0.05, the AMF uncertainty due to HS errors is relatively small, generally below 0.2%, while for AS = 0.8 it is further reduced to mostly below 0.01%. (2) The AMF uncertainty decreases with increasing surface elevation: low-elevation surfaces (0–1 km) exhibit higher sensitivity, particularly under polluted and volcanic degassing scenarios, whereas at high elevations (>5 km) the uncertainty becomes negligible (<0.02%). (3) The sensitivity to HS varies among different scenarios, which can be attributed to differences in the altitude of SO<sub>2</sub> concentration peaks in each profile.

### 5.2.4 Error source: SO<sub>2</sub> profile shape

Since the actual vertical distribution of atmospheric SO<sub>2</sub> is often difficult to obtain, a priori profiles from chemical transport models are commonly used in AMF calculations. For regions dominated by anthropogenic emissions, models such as GEOS-Chem and TM5 are widely applied to provide global SO<sub>2</sub> vertical profiles for AMF estimation, and uncertainties in these profiles can propagate into the total AMF.

In this study, SO<sub>2</sub> vertical profiles from GEOS-CF were used for AMF calculations. Keller et al. (2021) reported that GEOS-CF v1.0 systematically overestimates SO<sub>2</sub> concentrations owing to outdated emission inventories, with model biases

**Deleted:** Box-AMF increases as surface reflectance increases (Fig. 20d) due to higher reflectivity enhancing atmospheric multiple scattering, which increases the photon path length and thereby raises Box-AMF values. When LER surface reflectance changes from 0 to 1, the surface Box-AMF increases from 0.23 to 4.14, an increase of approximately 1700%. However, the increase of surface reflectance also changes the vertical shape of Box-AMF, shifting it from increasing with altitude to decreasing with altitude. Fig. 20e shows that the Box-AMF decreases with increasing terrain height, as higher surface elevation reduces the atmospheric column above the ground, leading to less scattering and decreased sensitivity. (Fahrland et al., 2020)...

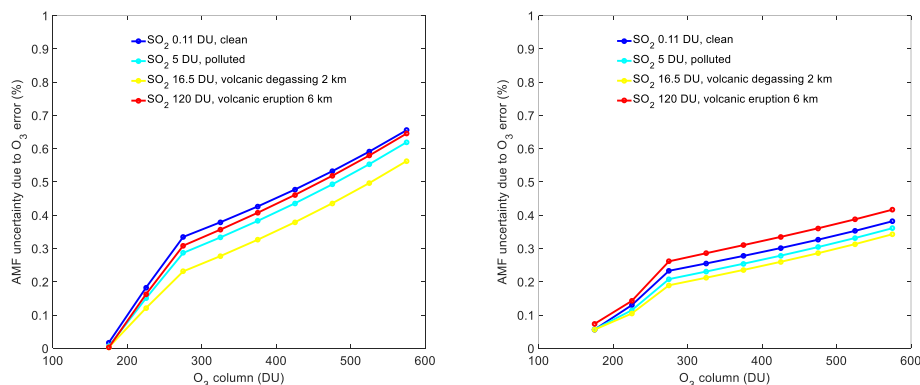
**Deleted:** The variation of Box-AMF with wavelength ranging from 310 nm to 330 nm (Fig. 20f) shows that Box-AMF increases with increasing wavelength. The difference in Box-AMF at different wavelengths varies with altitude. For example, near the surface, when the wavelength increases from 310 nm to 330 nm, the surface Box-AMF increases from 0.28 to 0.48, a rise of 71.13%; At an altitude of 10 km, the Box-AMF increases from 1.69 to 2.36, a rise of 39.57%. Note that for most cases in this study, the wavelength 320 nm, which is approximately at the center of the SO<sub>2</sub> retrieval window (312–326 nm), was chosen to perform the SCIATRAN Box-AMF calculation. The variation of Box-AMF with the O<sub>3</sub> column from 125 DU to 575 DU (Fig. 20g) shows that, compared to other influencing factors, O<sub>3</sub> column has a relatively weak impact on Box-AMF, especially for altitudes below 5 km. The Box-AMF gradually decreases as the O<sub>3</sub> column increases. The differences in Box-AMF under different O<sub>3</sub> column conditions are more noticeable between altitudes of 5 km and 25 km. For example, at an altitude of 15 km, Box-AMF decreases from 2.41 to 2.07 as the O<sub>3</sub> column increases from 125 DU to 575 DU, a decrease of about 14%....

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reaching up to a factor of four. However, at the time of writing, detailed information on the layer-resolved uncertainties and temporal biases of GEOS-CF SO<sub>2</sub> vertical profiles is not available. Considering that the GEOS-CF results originate from the GEOS-Chem chemistry module, the uncertainty estimates reported in Lee et al. (2009) were adopted, where the AMF uncertainty due to GEOS-Chem SO<sub>2</sub> profile errors was generally in the range of 10–22% under clear-sky conditions.

### 5.2.5 Error source: O<sub>3</sub>



**Figure 23:** AMF uncertainty due to O<sub>3</sub> errors for different scenarios. (Left) AS=0.05; (Right) AS=0.8.

The variation of Box-AMF with the O<sub>3</sub> column (Fig. 19g) shows that, O<sub>3</sub> column has a relatively weak impact on Box-AMF, especially for altitudes below 5 km. The Box-AMF gradually decreases as the O<sub>3</sub> column increases. The differences in Box-AMF under different O<sub>3</sub> column conditions are more noticeable between altitudes of 5 km and 25 km. In this study, the total O<sub>3</sub> column from OMS was used in the OMS SO<sub>2</sub> AMF calculation, with an estimated uncertainty of less than 5%. Assuming O<sub>3</sub> error of 5%, the estimate of AMF uncertainty due to O<sub>3</sub> errors is generally small (Fig. 23), with values below 0.7% for dark surfaces (AS = 0.05) and below 0.4% for bright surfaces (AS = 0.8). AMF uncertainty increases slightly with increasing O<sub>3</sub> total column, especially for dark surfaces.

### 5.2.6 Error source: wavelength dependence

The wavelength dependence of AMF is a non-negligible error source of AMF uncertainty. The variation of Box-AMF with wavelength ranging from 310 nm to 330 nm (Fig. 19f) shows that Box-AMF increases with increasing wavelength. In this study, the wavelength 320 nm, which is approximately at the center of the SO<sub>2</sub> retrieval window (312–326 nm), was selected for the AMF calculation. To evaluate the AMF uncertainty due to wavelength dependence, three representative wavelengths within the retrieval window (313 nm, 320 nm, and 325 nm) were selected to quantify the impact of wavelength dependence.

**Deleted:** (Keller et al., 2021) As seen from the above results, compared to other influencing factors, surface reflectance has a relatively strong impact on Box-AMF, thus affecting the accuracy of AMF calculations, especially in anthropogenic emission regions where SO<sub>2</sub> is concentrated near the surface. The errors of Box-AMF from surface reflectance primarily come from two aspects. One is the errors in the surface reflectance climatology. In many satellite products, for each pixel, a surface reflectance climatology (such as from OMI (Kleipool et al., 2008) or TROPOMI (Tilstra et al., 2024)) is interpolated to obtain the corresponding surface reflectance, which is then used as input to calculate the corresponding Box-AMF. The uncertainties in the surface reflectance climatology and interpolation errors due to the spatial resolution differences between the satellite observations and surface reflectance climatology can degrade the accuracy of the Box-AMF calculations. The sensitivity analysis of AS error on SCIATRAN Box-AMF (Fig. 21), which was conducted by introducing a 1% and 0.01 perturbation in AS values ranging from 0.01 to 0.90, shows that (1) The uncertainties in Box-AMF due to a 1% and 0.01 AS variation show a decreasing trend with increasing altitude, meaning that Box-AMF is more sensitive to AS at lower altitudes. (2) The uncertainties of Box-AMF due to a 1% AS variation increase as the AS increases, while those due to a 0.01 AS variation decrease as the AS increases. When AS is small (e.g., AS = 0.01, 0.03, 0.05), a 1% variation in AS can lead to less than a 0.5% change in Box-AMF near the surface. However, when AS ranges from 0.8 to 0.9, the uncertainties of Box-AMF due to a 1% AS variation can reach up to 1.1%–1.2% near the surface. Another aspect affecting the accuracy of Box-AMF due to surface reflectance is the assumption of surface reflectance as LER during SCIATRAN Box-AMF calculation. Surface reflectivity, which depends on the surface properties and the geometry of incident and reflected light, is not uniformly distributed in all directions (i.e., anisotropy). This anisotropy is typically described by the bidirectional reflectance distribution function (BRDF). However, due to more scattering in the UV, this effect is more relevant at longer wavelengths. Therefore, accurate AS input is crucial for the accuracy of Box-AMF calculation, especially in regions with high surface reflectance. Neglecting forward model errors, Figure 22 shows the dependence of AMF on SZA, VZA, AS, wavelength, O<sub>3</sub> column, and SO<sub>2</sub> profiles. The AMFs were calculated with SCIATRAN Box-AMFs using six assumed SO<sub>2</sub> profiles. Here six SO<sub>2</sub> profiles were constructed, representing clean conditions, low, medium, and high anthropogenic SO<sub>2</sub> emissions, volcanic degassing with plume heights around 2 km, and volcanic eruptions with plume heights around 6 km. As show

**Deleted:** In future work, we aim to incorporate high-resolution and satellite-synchronized SO<sub>2</sub> vertical profiles to improve the accuracy of AMF.

resolution satellite observations, it is often necessary to build a Box-AMF lookup table (LUT) by using radiative transfer model that considers variables such as SZA, VZA, RAA, AS, HS, wavelength, O<sub>3</sub> column, and cloud cover. The corresponding Box-AMF values for each satellite observation pixel are then obtained through interpolation within the LUT. This approach significantly improves the efficiency of retrieval, avoiding excessive computational time that would result from repeatedly running the radiative transfer model. However, the LUT approach may introduce new errors into the Box-AMF results. First, LUT are typically constructed based on specific atmospheric conditions and forward input parameters, which may not accurately represent real atmospheric conditions. Secondly, the interpolation process within the LUT introduces further uncertainties into the Box-AMF results.

As shown in Table 5, the AMF uncertainty due to wavelength dependence ranges from approximately 5.4% to 6.8% for dark surfaces ( $AS = 0.05$ ) and decreases to about 3.5%–4.5% for bright surfaces ( $AS = 0.8$ ). This indicates that AMF is more sensitive to wavelength variations under dark surface conditions, whereas enhanced multiple scattering over bright surfaces reduces the impact of wavelength dependence. Among the four scenarios, polluted conditions and volcanic degassing exhibit larger wavelength-related uncertainties, while clean and volcanic eruption cases show relatively lower sensitivity.

**Table 5. AMF uncertainty due to wavelength dependence**

	SO <sub>2</sub> profile, 0.11 DU,	SO <sub>2</sub> profile, 5 DU,	SO <sub>2</sub> profile, 16.5 DU,	SO <sub>2</sub> profile, 120 DU,
	clean	polluted	volcanic degassing	volcanic eruption
$AS=0.05$	5.43%	6.04%	6.82%	4.48%
$AS=0.8$	4.17%	4.36%	4.50%	3.54%

### 5.2.7 Error source: others

In addition to the error sources discussed above, other factors may also contribute to AMF uncertainty. However, their impacts on AMF have not yet been quantitatively assessed in this study. These factors include (1) uncertainties in the radiative transfer model, which are generally considered to be small; (2) interpolation errors. For SO<sub>2</sub> retrievals from high spatial resolution satellite observations, it is often necessary to construct a LUT using a radiative transfer model to improve retrieval efficiency. However, the LUT approach, which requires an interpolation process, may introduce additional uncertainties into the Box-AMF results.

### 5.2.8 Total AMF uncertainty

Overall, the AMF uncertainty is primarily dominated by uncertainties in surface reflectance, the SO<sub>2</sub> vertical profile shape, and wavelength dependence, while the contributions from ozone and terrain height are relatively small. Assuming that these error sources are independent, the total AMF uncertainty can be expressed as the quadrature sum of the AMF uncertainties due to surface reflectance ( $AS$ ), terrain height ( $HS$ ), SO<sub>2</sub> vertical profile shape  $S(z)$ , O<sub>3</sub> column, and wavelength dependence, as follows:

$$\sigma_{AMF} = \sqrt{\left(\frac{\partial AMF}{\partial AS} \sigma_{AS}\right)^2 + \left(\frac{\partial AMF}{\partial HS} \sigma_{HS}\right)^2 + \left(\frac{\partial AMF}{\partial S(z)} \sigma_{S(z)}\right)^2 + \left(\frac{\partial AMF}{\partial O_3} \sigma_{O_3}\right)^2 + \left(\frac{\partial AMF}{\partial \lambda} \sigma_{\lambda}\right)^2}$$

The total AMF uncertainties under five scenarios—clean, boundary layer pollution, boundary layer pollution over snow and ice, volcanic degassing, and volcanic eruption—are estimated to be 12–23%, 13–24%, 11–22%, 14–24%, and >50%, respectively. It should be noted that these values were calculated under clear-sky conditions, without considering the effects of clouds or aerosols.

**Table 6. OMS SO<sub>2</sub> AMF uncertainty due to individual error components under different clear-sky scenarios**

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Error source	Parameter uncertainty	Clean	Boundary layer pollution	Boundary layer pollution over snow and ice	Volcanic degassing	Volcanic eruption
Surface reflectance	0.02	~4%	~6%	~2%	~6%	~2%
Terrain height	4 m	~0.07%	~0.08%	~0.004%	~0.12%	~0.04%
SO <sub>2</sub> vertical profile shape	=	10–22%	10–22%	10–22%	10–22%	Large(>50%)
O <sub>3</sub> column	<5%	~0.3%	~0.3%	~0.2%	~0.2%	~0.3%
Wavelength dependence	=	~5%	~6%	~4%	~7%	~4%
<b>Total uncertainty of OMS SO<sub>2</sub> AMF</b>		<b>12–23%</b>	<b>13–24%</b>	<b>11–22%</b>	<b>14–24%</b>	<b>&gt;50%</b>

### 5.3 Errors from background offset correction

Background offset correction is essential for the OMS SO<sub>2</sub> column retrievals which have obvious along-track stripes and cross-track asymmetries problems. However, it is hard to get the accurate background offset for SO<sub>2</sub> retrieval of each pixel. In this study, an iterative sliding correction scheme for background offset correction was applied to OMS SO<sub>2</sub> retrievals, with the purpose of forcing SO<sub>2</sub> values over clean or low SO<sub>2</sub> emission regions to zero. This approach helps addressing problems such as along-track stripes and cross-track asymmetry. However, the sliding window strategy assumes that pixels with values smaller than the threshold (2 DU) within the sliding window represent zero SO<sub>2</sub> emissions, which may lead to a loss of SO<sub>2</sub> information contained in the low-emission regions. This not only could limit the applicability of the OMS SO<sub>2</sub> product for monitoring anthropogenic emission sources, but also may lead to many negative retrievals of SO<sub>2</sub> column in clean regions. Furthermore, SO<sub>2</sub> retrievals at certain cross-track positions (assumed to be clean near-zero) may exceed the 2 DU threshold, requiring the threshold to be adjusted upwards to achieve a better effect after background offset correction. Therefore, although the current background offset correction strategy helps mitigate stripes, residual systematic errors may still remain after the correction, which could affect the accuracy of the OMS SO<sub>2</sub> column retrievals.

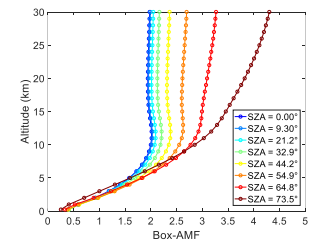
The quantification of the residual systematic errors is challenging, as it is difficult to fully separate random fitting errors from residual systematic components. Therefore, in this study, the residual systematic errors after the background offset correction were combined with the random fitting errors and treated as an effective SCD uncertainty, which was subsequently used in the total uncertainty estimation of the OMS SO<sub>2</sub> VCD.

### 5.4 Total uncertainty of OMS SO<sub>2</sub> VCD

In general, assuming that the error sources are independent of each other, the uncertainty of satellite-retrieved SO<sub>2</sub> VCD can be estimated using the following standard error propagation approach (Lee et al., 2009; Theys et al., 2017):

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$$\sigma_{SO_2} = \sqrt{\left(\frac{\sigma_{SCD}}{AMF}\right)^2 + \left(\frac{\sigma_{SCD}^{back}}{AMF}\right)^2 + \left(\frac{(SCD-SCD^{back}) \cdot \sigma_{AMF}}{AMF^2}\right)^2} \quad \text{(Eq. 4)}$$

where  $\sigma_{SCD}$  is the random error from DOAS  $SO_2$  SCD spectral fitting including instrument-related noise,  $\sigma_{SCD}^{back}$  is the residual systematic error after background offset correction, and  $\sigma_{AMF}$  is the AMF uncertainty which includes two components: one is related to the atmospheric scattering weight and the other one is associated with the  $SO_2$  profile shape.

In the standard error propagation method,  $\sigma_{SCD}$  is commonly approximated by the SFE. However, for the OMS  $SO_2$  retrieval, the SFE is strongly affected by instrument-related systematic errors, as shown in Fig. 18. As a result, the SFE includes not only random fitting errors but also systematic components, and thus does not represent the random SCD uncertainty. If directly used as  $\sigma_{SCD}$  in the error propagation, it would lead to an overestimation of the total uncertainty of the OMS  $SO_2$  VCD.

Therefore, the SFE was not adopted as  $\sigma_{SCD}$  in this study. Instead, the standard deviation of the corrected SCD over clean oceanic regions, approximately 0.2 DU in equatorial regions and about 0.4 DU at high latitudes, was used as an effective SCD uncertainty. This value reflects the combined effect of random fitting error and residual systematic errors after background offset correction and was propagated into the total uncertainty estimation. Accordingly, the total uncertainty of the OMS  $SO_2$  VCD can be expressed as:

$$\sigma_{SO_2} = \sqrt{\left(\frac{\sigma_{SCD,res}}{AMF}\right)^2 + \left(\frac{SCD_{corr} \cdot \sigma_{AMF}}{AMF^2}\right)^2} \quad \text{(Eq. 5)}$$

where  $\sigma_{SCD,res}$  is the effective SCD uncertainty, and  $SCD_{corr}$  is the background-corrected  $SO_2$  SCD.

The estimated total uncertainties of OMS  $SO_2$  VCDs under four scenarios—clean, boundary layer pollution, volcanic degassing, and volcanic eruption—are summarized in Table 7. The results show that under clean conditions, the total uncertainty is dominated by measurement noise and fitting errors, ranging from 0.16–0.17 DU at low latitudes and 0.32–0.33 DU at high latitudes. The corresponding relative errors are ~150% at low latitudes and ~295% at high latitudes, reflecting the challenge of retrieving low  $SO_2$  column. For boundary layer pollution scenarios, the enhanced  $SO_2$  signal reduces the relative errors to 14–25%, while the total uncertainty increases to 0.68–1.21 DU at low latitudes and 0.75–1.26 DU at high latitudes. For volcanic degassing, the relative errors range from 14–24%, with total uncertainties ranging from 2.32 to 3.97 DU. Under the volcanic eruption scenario, the total uncertainty and relative error are approximately 60 DU and 50%, respectively. It should be noted that these estimates still involve large uncertainties due to the large errors in radiance measurement and  $SO_2$  vertical profile provided by GEOS-CF, particularly under volcanic eruption conditions. In addition, the uncertainties associated with clouds and aerosols were not included in the present error analysis, suggesting that the estimated uncertainties may be conservative.

**Table 7. Total uncertainty of OMS  $SO_2$  VCDs under different clear-sky scenarios**

Scenario	Total uncertainty (DU)	Relative error (%)
Clean	Low latitude: 0.16–0.17 DU High latitude: 0.32–0.33 DU	Low latitude: ~150% High latitude: ~295%
Boundary layer pollution	Low latitude: 0.68–1.21 DU High latitude: 0.75–1.26 DU	Low latitude: 14–25% High latitude: 15–25%
Volcanic degassing	2.32–3.97 DU	14–24%
Volcanic eruption	~60 DU	~50%

## 6 Conclusions and future work

This study presents the first SO<sub>2</sub> retrieval results from the Chinese FY-3F/OMS instrument, which was launched in August 2023. The results were derived using TOA reflected radiance data from FY-3F/OMS with a DOAS approach. To improve the retrieval accuracy, specific processing schemes were developed based on the characteristics of the OMS instrument and the performance of its L1 data. These schemes, including solar spectrum selection, spectral soft calibration, and background offset correction, effectively reduce along-track stripes and across-track asymmetry in the OMS SO<sub>2</sub> retrievals.

To evaluate the accuracy of OMS SO<sub>2</sub> retrievals, comparisons with TROPOMI DOAS and TROPOMI COBRA SO<sub>2</sub> products were conducted over clean oceanic regions, volcanic eruptions, and 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 SO<sub>2</sub> emissions from volcanic eruptions and anthropogenic sources. In selected clean oceanic regions, the SO<sub>2</sub> 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, FY-3F/OMS SO<sub>2</sub> retrievals successfully capture the spatial distribution and high-concentration plumes of volcanic SO<sub>2</sub>, similar to the TROPOMI DOAS and TROPOMI COBRA 7 km SO<sub>2</sub> results. However, OMS tends to underestimate SO<sub>2</sub> at high columns (>50 DU) due to saturation in the 312–326 nm fitting window. In anthropogenic emission regions, OMS and TROPOMI SO<sub>2</sub> products show generally good consistency in detecting anthropogenic SO<sub>2</sub> emissions, with correlation coefficients ranging from about 0.6–0.9 over the Persian Gulf and 0.80–0.85 over Norilsk. The differences between OMS and TROPOMI SO<sub>2</sub> 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, SO<sub>2</sub> retrieval fitting windows, AMF strategies).

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. With its high spectral and spatial resolution, morning overpass time, daily global coverage, and reliable SO<sub>2</sub> retrieval results, OMS will provide effective data

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**Deleted:** Among these, the AMF used in the SO<sub>2</sub> column retrieval is a major contributor to the differences between OMS and TROPOMI SO<sub>2</sub> results. For example, in the case of the Sundhnúkur volcano, the lack of accurate information on the vertical SO<sub>2</sub> profile can lead to discrepancies of more than a factor of two when comparing the OMS and TROPOMI SO<sub>2</sub> results. Random noise and uncertainties from background correction are relevant for low SO<sub>2</sub> 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. ...

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support for monitoring the continuous SO<sub>2</sub> changes from global volcanic eruptions and anthropogenic activities, helping to fill the spatial and temporal gaps in the existing global satellite network.

185 The current OMS SO<sub>2</sub> retrievals still have several shortcomings that need to be addressed in the future. More work will be needed to incorporate accurate and satellite-synchronized SO<sub>2</sub> vertical profiles to improve the accuracy of AMF. In addition, higher spatial resolution surface reflectance products that account for directional effects, as well as the impacts of clouds and aerosols on the AMF, should be considered in the OMS SO<sub>2</sub> AMF calculation. Another issue that needs to be addressed in the future is the simultaneous retrieval of volcanic eruption heights, which would help improve the accuracy of SO<sub>2</sub> retrievals in volcanic regions. Moreover, the 312–326 nm retrieval fitting window used in the OMS SO<sub>2</sub> product exhibits nonlinear variation in the case of very large SO<sub>2</sub> concentrations, leading to an underestimation of SO<sub>2</sub> columns. In the future, SO<sub>2</sub> retrievals from longer UV wavelength fitting windows varying with SO<sub>2</sub> columns will be incorporated into the OMS SO<sub>2</sub> retrieval to mitigate the saturation issue in the case of large volcanic eruptions. Our preliminary strategy for such retrievals is as follows. First, a global SO<sub>2</sub> 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.

Furthermore, although in this study the comparison between OMS SO<sub>2</sub> retrievals and TROPOMI SO<sub>2</sub> products was conducted to demonstrate the capability of OMS SO<sub>2</sub> retrievals, synchronous and high-quality ground-based or airborne measurements remain crucial for validating the accuracy of OMS SO<sub>2</sub> retrievals. In the future, ground-based and airborne experiments need to be conducted to provide accurate ground-based or airborne data for the validation of OMS SO<sub>2</sub> retrievals.

#### 2205 Author contribution

HY: Drafting, data processing, and plotting; AR: Revision, research methodology and content suggestions, and English polishing; XZ: Suggestions on revision and research direction; AS: Discussion and suggestions on the Ring effect; TY & YL & CY: Discussion and suggestions on AMF calculation; QW: Discussion on the data quality of OMS L1 data; LZ & WW: Discussion and suggestions on the revision of the Error analysis section.

#### 2210 Data Availability

The SO<sub>2</sub> data produced in this study is available from the authors on request. FY-3F/OMS-N L1 data can be downloaded from the website <http://data.nsmc.org.cn/DataPortal/en/home/index.html>. TROPOMI DOAS SO<sub>2</sub> data is available via the

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2230 Copernicus Data Space Ecosystem (<https://browser.dataspace.copernicus.eu/>). TROPOMI COBRA SO<sub>2</sub> data is available via the PAL system (<https://data-portal.s5p-pal.com/products/so2cbr.html>).

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