Making **Ea**rth **S**cience Data Records for **U**se in **R**esearch **E**nvironment**s** (MEaSUREs)

README Document for

OMPS_NPP_NMSO2_PCA_L2

OMPS NPP Nadir Mapper SO_2 Level 2 Product

Based on PCA Algorithm

Goddard Earth Sciences Data and Information Services Center (GES DISC)

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Revision History

09/13/2019, NMSO2_PCA_L2 product updated from version 1.1 (V1.1) to version 1.2 (V1.2), introducing a new volcanic SO_2 flagging scheme.

07/28/2020, NMSO2_PCA_L2 product updated from version 1.2 (V1.2) to version 2.0 (V2.0), introducing a new anthropogenic SO_2 dataset consistent with Aura/OMI OMSO2 version 2.0 product.

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1. INTRODUCTION

1.1 OMPS_NPP_NMSO2_PCA_L2 Product

This document describes the OMPS_NPP_NMSO2_PCA_L2 data product (henceforth shortened to NMSO2_PCA_L2). NMSO2_PCA_L2 is a Level 2, orbital-track volcanic and anthropogenic sulfur dioxide (SO_2) product for the Ozone Mapping and Profiler Suite (OMPS) Nadir Mapper (NM) onboard the NASA/NOAA Suomi National Polar-orbiting Partnership (SNPP) satellite, which was launched on October 28, 2011 into a polar sun-synchronous orbit and has been collecting science data since January 2012. As part of the NASA's Making Earth System Data Records for Use in Research Environments (MEaSUREs) program and the SNPP Science Team program, the Goddard Earth Science (GES) Data and Information Data Center (DISC) has released a new SO_2 Earth System Data Record (ESDR), NMSO2_PCA_L2, processed using the Goddard Space Flight Center (GSFC) Principal Component Analysis (PCA) trace gas retrieval algorithm. NMSO2_PCA_L2 is a Level 2 orbital swath product that spans the entire SNPP/OMPS record. It offers great consistency with the NASA Earth Observing System (EOS) Aura/OMI (Ozone Monitoring Instrument, launched in 2004) SO_2 product (OMSO2, https://doi.org/10.5067/Aura/OMI/DATA2022) produced with the same PCA algorithm, and provides continuity between OMI and the follow-up OMPS instruments aboard the NASA/NOAA JPSS satellites.

1.2 OMPS/SNPP Nadir Mapper

The Nadir Mapper (NM) of OMPS is a nadir-viewing UV spectrometer that measures backscattered solar UV radiance spectra from the Earth and solar irradiance in the 300–380 nm wavelength range at a spectral resolution of ~1 nm (Flynn et al., 2014; Seftor et al., 2014). The first model has been flying onboard the NASA/NOAA SNPP spacecraft since 2011, in a sun-synchronous orbit with a local afternoon equator crossing time of roughly 1:30 p.m. OMPS-NM has a 110° field of view (FOV) and covers a cross-track swath of approximately 2800 km, providing global coverage on a daily basis (14-15 orbits per day). The nominal spatial resolution of OMPS-NM is 50 km × 50 km at nadir in the nominal observation mode. For about one day every week, the instrument takes measurements in the high spatial resolution mode but at fewer wavelengths. Currently, NMSO2_PCA_L2 data are limited to the nominal observation mode.

1.3 Science Background

SO_2 is an important air pollutant that has significant impacts on both air quality and climate. It is emitted from both anthropogenic sources (*e.g.*, power plants) and volcanoes. Oxidation of SO_2 in the atmosphere produces secondary sulfate aerosols, a major compound responsible for acid deposition and smog and haze. By scattering solar radiation and acting as cloud condensation nuclei, sulfate aerosols also directly and indirectly alter the radiation budget of the Earth.

Satellite retrievals of SO_2 began with Nimbus-7 Total Ozone Mapping Spectrometer (TOMS, Kruger 1983). With measurements only at six discrete wavelengths, the TOMS SO_2 data record is generally limited to large volcanic eruptions (Fisher *et al.*, 2019). Starting from the 1990s, hyperspectral UV measurements made by instruments such as GOME (Global Ozone Monitoring Experiment) allow SO_2 absorption features to be more clearly separated from interfering processes, enabling the detection of anthropogenic SO_2 signals from space (*e.g.*, Eisinger and Burrows, 1998). Since 2004, the Dutch-Finnish Ozone Monitoring Instrument (OMI) onboard NASA's polar orbiting Aura satellite has been providing global monitoring of both anthropogenic and volcanic SO_2 with increased spatial resolution. The previous NASA standard OMI SO_2 product is based on discrete wavelength Band Residual Difference (BRD, Krotkov *et al.,* 2006) and Linear Fit (LF, Yang *et al*., 2007) algorithms. The new generation standard OMI SO_2 product (first released in 2014, updated in 2016 and 2020) is based on the Principal Component Analysis (PCA) algorithm (Li *et al*., 2013; 2017; 2020) that offers significantly improved data quality. NMSO2_PCA_L2 is produced with the same PCA retrieval algorithm that has been implemented for Aura/OMI.

2. PRINCIPAL COMPONENT ANALYSIS SO_2 ALGORITHM

2.1 General Description

This section describes the Principal Component Analysis (PCA) SO_2 algorithm and its implementation with SNPP/OMPS. The algorithm has been described in detail elsewhere (Li *et al.*, 2013; 2017; 2020) and is only briefly summarized here. In this algorithm, we apply a PCA technique to satellite measured backscattered UV (BUV) radiances between ~310 and 340 nm to extract spectral features from the measured spectra. These features, in the form of Principal Components (PCs), are related to various geophysical processes (*e.g.*, ozone absorption, rotational Raman scattering) and instrument measurement details (*e.g.*, wavelength shift, dark current). We use these PCs in SO_2 spectral fitting to reduce their interferences. It should be noted that BUV instruments such as OMI and OMPS have different sensitivities to SO_2 at different altitudes. In the absence of such information on the SO_2 plume height, for each OMPS pixel, the NMSO2_PCA_L2 provides six estimates of the total SO_2 Vertical Column Density (VCD) in Dobson Units (1 DU = 2.69 $\cdot 10^{16}$ molecules/cm^2), corresponding to different assumed *a priori* profiles or Center of Mass Altitude (CMA). All six VCD values represent the estimated total number of SO_2 molecules within the entire atmospheric column (in DU or molecules/cm^2). Therefore, they should not be interpreted as partial column amounts within different vertical layers of the atmosphere. The six estimates are provided so that data users may select the estimate that is best suited for the case of interest. Additionally, for anthropogenic SO_2, users have the option to use their own *a priori* SO_2 vertical profiles (see section 2.2 for details).

2.2 Anthropogenic SO_2 Retrieval (Updated in Version 2.0)

For studies on anthropogenic SO_2 pollution, we recommend the use of anthropogenic SO_2 dataset (data field name: ColumnAmountSO2) in the NMSO2_PCA_L2 V2.0 product. Over areas with relatively large anthropogenic sources such as coal-fired power plants or metal smelters, SO_2 is generally more concentrated within the planetary boundary layer (PBL) or approximately the lowest 1-2 km of the atmosphere. On the other hand, SO_2 mixing ratio within the PBL is usually quite low (much less than 1 ppb, parts per billion, 10^{-9}) over relatively clean background areas (*e.g.*, the remote Pacific Ocean). The PBL SO_2 dataset (data field name: ColumnAmountSO2_PBL) in the earlier versions of NMSO2_PCA_L2 (V1.2 and earlier) contains estimates of SO_2 VCDs assuming that SO_2 is predominantly in the PBL everywhere, including over background regions. Starting from NMSO2_PCA_L2 V2.0, we introduce the new ColumnAmountSO2 dataset that uses updated Jacobian lookup tables and model-based *a priori* SO_2 profile shapes (see below and section 2.6 for details). With these updates, ColumnAmountSO2 has improved data quality and should be used in place of the old ColumnAmountSO2_PBL dataset from the previous versions of NMSO2_PCA_L2 for air quality studies.

Despite various updates to the Jacobian calculations, the NMSO2_PCA_L2 V2.0 algorithm shares the same overall framework with the V1.2 algorithm. For each OMPS orbit, we process its 36 rows (cross-track positions) one at a time, employing a PCA technique to extract Principal Components (PCs or v_i) from the sun-normalized BUV radiance spectra in the wavelength range of 310.5-340 nm. The PCs are ranked in descending order according to the spectral variance they each explain. If derived from SO_2-free regions, the first several PCs that account for most of the variance are representative of geophysical processes unrelated to SO_2 such as ozone (O_3) absorption, as well as measurement details such as wavelength shift. We then obtain an estimate of SO_2 VCD (Ω_{SO2}) and the coefficients of the PCs (**ω**) by fitting the first n_v (up to 20 non-SO_2) PCs and the SO_2 Jacobians ($\partial N/\partial\Omega_{SO_2}$) to the measured radiance spectrum (in this case the quantity N, which is the scaled logarithm of the sun-normalized radiances, I):

$$N(\omega, \Omega_{SO_2}) = \sum_{i=1}^{n_v} \omega_i v_i + \Omega_{SO_2} \frac{\partial N}{\partial \Omega_{SO_2}}. \quad (1)$$

The SO_2 Jacobians represent the sensitivity of sun-normalized BUV radiances (I or its logarithm, N) at the Top Of Atmosphere (TOA) to a unit perturbation in Ω_{SO2}, and were pre-calculated with the VLIDORT radiative transfer code (Spurr, 2008). The previous versions of NMSO2_PCA_L2 (V1.2 and earlier) algorithm use a fixed SO_2 Jacobian spectrum in eq. (1) for PBL SO_2 retrievals, calculated assuming that SO_2 is predominantly in the lowest 1 km of the atmosphere and that the observation is made under cloud-free conditions with fixed surface albedo (0.05), surface pressure (1013.25 hPa), solar zenith angle (30°), viewing zenith angle (0°), and pre-set O_3 and temperature profiles (with O_3 VCD = 325 DU). These simplified assumptions do not account for the pixel-to-pixel changes in the actual observational conditions and can lead to relatively large biases particularly for cloudy pixels or pixels near the edges of the OMPS swath.

For the new anthropogenic SO_2 dataset (ColumnAmountSO2) in NMSO2_PCA_L2 V2.0, we use a table lookup approach to estimate SO_2 Jacobian/air mass factor (AMF) for each individual OMPS pixel. Scattering weight or vertically resolved box-AMF is defined as:

$$m(z) = -\frac{\partial ln(I)}{\partial \tau_{SO2}(z)}. \quad (2)$$

It represents the sensitivity of OMPS measured TOA radiances (I) to changes in SO_2 optical thickness, τ_{SO2}, at a given altitude (or pressure level) z. Scattering weight depends on O_3 (both the amount and vertical profile), solar and viewing zenith angles (θ_0 and θ), the relative azimuth angle (ϕ), and the pressure and reflectivity (R) of the underlying clouds or surfaces. The scattering weight is interpolated from the Jacobian lookup tables following eq. (3):

$$m(z) = \left[\frac{\partial I_0(\theta_0,\theta)}{\partial\tau_{so2}(z)} + \frac{\partial I_1(\theta_0,\theta)}{\partial\tau_{so2}(z)}\cos\phi + \frac{\partial I_2(\theta_0,\theta)}{\partial\tau_{so2}(z)}\cos 2\phi + \frac{R}{(1-RS_b)}\frac{\partial I_r(\theta_0,\theta)}{\partial\tau_{so2}(z)} + \frac{R^2 I_r(\theta_0,\theta)}{(1-RS_b)^2}\frac{\partial S_b}{\partial\tau_{so2}(z)}\right]\cdot I^{-1}\,, \tag{3}$$

where I_0, I_1, and I_2 represent the atmospheric contribution to the radiances (I). RI_r represents the TOA radiance that is reflected once from the surface and transmitted through the atmosphere, and ($1 - RS_b$) accounts for the effects of multiple reflections between the surface and the atmosphere, with S_b being the fraction of the Lambertian surface-reflected radiation that is scattered back to the surface by the atmosphere.

To build the Jacobian lookup tables, we ran the VLIDORT radiative transfer code to compute scattering weights at eight solar zenith angles (θ_0: 0-81°), eight viewing zenith angles (θ: 0-80°) defined at the bottom of atmosphere, and six nodes for the underlying surface/cloud pressures (240-1013 hPa) for each of the 46 ozone climatology profiles from Labow *et al.* (2015). The scattering weights at 72 vertical layers (0.01-1013.25 hPa) were calculated at 801 wavelengths between 305 and 345 nm at 0.05 nm resolution, leading to a Jacobian lookup table with dimensions of 6 × 8 × 8 × 72 × 801 for each ozone climatology profile.

For each OMPS pixel, we use the effective cloud fraction (f_c) and optical centroid pressure (OCP) from the NMCLDRR product [Vasilkov *et al.*, 2014] to estimate the scattering weights under overcast conditions ($m_{cld}(z)$, $f_c = 1$). We also estimate the scattering weights ($m_{cld}(z)$) under cloud free conditions ($m_{clr}(z)$, $f_c = 0$), and calculate the weighted average between cloudy and cloud-free scattering weights using the cloud radiance fraction (CRF) for the pixel:

$$m(z) = m_{cld}(z)CRF + m_{clr}(z)(1 - CRF), \tag{4}$$

$$CRF = f_c\frac{I_{cld}}{I_{meas}}, \tag{5}$$

where I_{cld} and I_{meas} are the calculated radiances with $f_c = 1$ and the measured radiances at TOA, respectively.

The column air mass factor (AMF) for the pixel can then be calculated from the scattering weights and the *a priori* profile shape of SO_2, $n_{SO2}(z)$:

$$AMF = \int_0^{TOA} m(z)\, n_{SO2}(z)dz\,, \tag{6}$$

where $n_{SO2}(z)$ is unitless and represents the fraction of SO_2 molecules contributed by layer z to the overall SO_2 molecules within the entire atmospheric column.

In NMSO2_PCA_L2 V2.0 anthropogenic SO_2 retrievals, we estimate the column SO_2 Jacobians at all wavelengths between 310.5 and 340 nm and use the Jacobian spectra in fitting to estimate the SO_2 VCDs based on eq. (1). We also provide the SO_2 slant column densities (SCDs, data field name: SlantColumnAmountSO2) by fitting the PCs and the cross sections of SO_2 to the measured radiances. The SCD for an OMPS pixel can be converted to VCD using the *AMF*:

$$VCD = \frac{SCD}{AMF}. \quad (7)$$

In NMSO2_PCA_L2 V2.0, SCD is provided along with the scattering weight profile at 313 nm for each OMPS pixel. Data users can apply their own *a priori* profiles to obtain updated estimates of AMFs and VCDs following eqs. (6) and (7).

For *a priori* profile shapes ($n_{SO2}(z)$ in eq. 6), we use monthly climatology profiles built from a set of GEOS-5 (Goddard Earth Observing System, Version 5) global model simulations (72 vertical layers, 0.5° latitude by 0.667° longitude horizonal resolution) for the period of 2004-2014. The *a priori* profile shape of SO_2 ($n_{SO2}(z)$) used for each OMPS pixel is provided in the data field GEOS5LayerWeight in NMSO2_PCA_L2 V2.0.

In addition to retrievals with GEOS-5 based *a priori* profiles, we also estimate SO_2 VCDs using the same Jacobian lookup table, but different *a priori* profiles that assume constant SO_2 mixing ratio within the lowest 1 km of the atmosphere and negligible SO_2 above 1 km. The resulting dataset (ColumnAmountSO2_PBL) is independent of the GEOS-5 simulations and can be useful for top-down emission estimates. ColumnAmountSO2_PBL is retrieved for each OMPS pixel with CRF < 0.5, and the corresponding *a priori* profile shape with zero weights above 1 km (data field name: PBLLayerWeight) is also provided in NMSO2_PCA_L2 V2.0.

2.3 Volcanic SO_2 Retrieval

To facilitate studies on volcanic SO_2, NMSO2_PCA_L2 provides SO_2 VCD estimates assuming SO_2 plume heights or CMAs of 3 (lower troposphere, TRL), 8 (middle troposphere, TRM), 13 (upper troposphere, TRU), and 18 (lower stratosphere, STL) km. The first two assumed CMAs are typical of volcano degassing and moderate eruptions, respectively, whereas the latter two represent explosive volcanic eruptions. For volcanic SO_2 retrievals, we use the SO_2 SCD (section 2.2) and the Simple Lambertian Equivalent surface Reflectivity (SLER or *R*) derived from TOA radiances for each pixel as input. Following the same parameterization as in eq. (3), the volcanic SO_2 Jacobians as a function of solar zenith angle (θ_0), viewing zenith angle (θ), and relative azimuth angle (ϕ) can be calculated with the following equation:

$$\frac{\partial I}{\partial \Omega_{so2}} = \frac{\partial I_0(\theta_0,\theta)}{\partial \Omega_{so2}} + \frac{\partial I_1(\theta_0,\theta)}{\partial \Omega_{so2}} \cos\phi + \frac{\partial I_2(\theta_0,\theta)}{\partial \Omega_{so2}} \cos 2\phi + \frac{R}{(1-RS_b)} \frac{\partial I_r(\theta_0,\theta)}{\partial \Omega_{so2}} + \frac{R^2 I_r(\theta_0,\theta)}{(1-RS_b)^2} \frac{\partial S_b}{\partial \Omega_{so2}} . \quad (8)$$

In the retrieval algorithm, the SO_2 Jacobians are interpolated from a set of pre-calculated lookup tables for 21 climatology O_3 profiles and four presumed SO_2 profiles (*i.e.*, TRL, TRM, TRU, and STL). The nodes of θ_0 (SZA), θ (VZA) and SO_2 in the volcanic SO_2 Jacobian lookup table are given in Table 1.

Table 1. Nodes of the Solar Zenith Angle (SZA), Viewing Zenith Angle (VZA), and SO_2 column amount, as used in the pre-computed SO_2 Jacobians lookup tables.

Parameter	Nodes														
SZA	0°		15°		30°		45°		60°		70°		77°		81°
VZA	0°		15°		30°		45°		60°		70°		75°		80°
SO_2 (DU)	0	1	5	10	50	100	200	300	400	500	600	700	800	900	1000

For each OMPS pixel, the SO_2 Jacobians are first calculated from the exact observational geometry, scene reflectivity, *R*, and SO_2 SCD (converted to VCD with an AMF = 0.36) for an initial estimate of the volcanic SO_2 VCD. Next, the SO_2 VCD from the first step is used as an input to the lookup table to obtain updated estimates for SO_2 Jacobians and VCD. The iterations continue until the results converge (SO_2 VCD difference between two successive steps < 0.1 DU or 1% for pixels with SO_2 VCD > 100 DU) or the number of iterations exceeds the upper limit (20). The retrieval starts from a nominal fitting window of 313-340 nm. But for pixels with strong SO_2 signals (*e.g.*, large eruptions), the fitting window is optimized for each iteration step to exclude shorter wavelengths that are saturated (*i.e.*, SO_2 Jacobians become significantly smaller with increasing SO_2 VCD). This optimal fitting window helps to reduce the interpolation error in SO_2 Jacobians and also the low bias in LF retrievals. The same data processing steps are applied separately for the TRL, TRM, TRU, and STL SO_2 VCD retrievals.

2.4 Data Quality Assessment and Data Filtering

Errors in NMSO2_PCA_L2 data can arise from both the input radiance data and the SO_2 Jacobians used in retrievals. We estimate the retrieval noise by calculating the standard deviation over presumably SO_2-free remote regions (*e.g.*, the equatorial Pacific). We have also conducted extensive comparisons between the NMSO2_PCA_L2 and the OMI PCA SO_2 data, and have found generally good agreement between the two products (Li et al., 2017; Zhang et al., 2017), despite large differences in instrument characteristics.

For data analysis, we recommend that all pixels with large solar zenith angles (SZA > 70°) or near the edge of the swath (rows 0-1 and 34-35, 0-based) or potentially affected by the South Atlantic Anomaly (Flag_SAA = 1) be excluded. There are also occasional stripes (unphysical, large positive or negative values for a large portion of a row) due to retrieval artifacts, and those affected pixels should be excluded in data analysis.

SlantColumnAmountSO2 (new in NMSO2_PCA_L2 V2.0): we can estimate the retrieval noise by calculating the pixel-level spatial standard deviation (σ) over background areas. The typical 1-σ noise over the presumably SO_2-free remote Pacific is ~0.1 DU or smaller at SZAs < 50° and ~0.2-0.3 DU at SZAs of 50-70°.

SlantColumnAmountSO2 can be used as a continuity product for our previous PBL SO_2 dataset (ColumnAmountSO2_PBL in NMSO2_PCA_L2 V1.2 and earlier) when a fixed AMF = 0.36 is applied. For best data quality, use data from pixels near the center of the swath (rows 2-33, 0-based) with small SZAs (< 65°) and CRF < 0.3. SlantColumnAmountSO2 retrievals for OMPS pixels from the descending node of the SNPP satellite should not be used.

ColumnAmountSO2 (new in NMSO2_PCA_L2 V2.0): The 1-σ noise of ColumnAmountSO2 is typically < 0.05 DU over remote oceanic areas, as SO_2 is usually more abundant at higher altitudes in the typical *a priori* profiles used for those areas, resulting in larger AMFs and lower noise in VCDs. Over land, the AMFs are generally smaller due to different *a priori* profile shapes, leading to greater noise in ColumnAmountSO2 particularly over polluted areas.

The SO_2 retrieval accuracy is also affected by multiple sources that may cause errors in the Jacobians/AMFs, including: 1) errors from forward radiative transfer model assumptions and the table lookup interpolation scheme; 2) errors in *a priori* profiles; 3) errors in input data such as cloud pressure, cloud fraction, and surface reflectivity; and 4) the lack of explicit correction for the effects of aerosols on Jacobians. Assuming all these sources of errors are independent, the overall relative uncertainty of AMF/Column Jacobians would be ~50-100% for a typical pixel over polluted areas (see Li et al., 2020 for more details).

As with SlantColumnAmoutnSO2, when using ColumnAmoutnSO2, it is recommended that data users exclude pixels in the outermost rows (0 and 35, 0-based), or with large cloud radiance fractions (CRF > 0.5), or with large solar zenith angles (> 70°). For best data quality, use data from pixels near the center of the swath (rows 2-33, 0-based) with SZA < 65°, CRF < 0.3, and AMF > 0.3. Pixels from the descending node of the SNPP satellite should not be used.

ColumnAmountSO2_PBL (updated in NMSO2_PCA_L2 V2.0): starting from V2.0, ColumnAmountSO2_PBL in the NMSO2_PCA_L2 product is no longer produced using the fixed Jacobian spectrum as in previous versions (V1.2 and earlier). Instead, the dataset is now produced using the same Jacobian lookup tables as in ColumnAmountSO2, but with different a priori profiles assuming that essentially all the SO_2 is in the lowest 1 km of the atmosphere. The noise in ColumnAmountSO2_PBL is generally greater than that in ColumnAmountSO2, especially over remote background areas. ColumnAmountSO2_PBL is intended for use in studies that aim to estimate the emissions from point sources. For best data quality, the same data screening criteria as those for ColumnAmountSO2 are recommended.

ColumnAmountSO2_TRL: Due to increased sensitivity to elevated SO_2, the pixel-level standard deviation in TRL data is estimated at ~0.1 DU under optimal observational conditions in the tropics. The noise is about 0.15 DU at high latitudes. The data can be used for cloudy, clear and mixed scenes as well as for elevated terrain, but will overestimate SO_2 VCDs if the SO_2 plume altitude is higher than 3 km. The TRL data can be used for studies on degassing volcanoes.

ColumnAmountSO2_TRM: The standard deviation of TRM retrievals over background areas is generally < 0.1 DU. Like the TRL data, the TRM data can be used for various sky conditions. The TRM data can be used for investigating SO_2 plumes from moderate eruptions, but will overestimate SO_2 VCDs if the SO_2 plume altitude is higher than ~8 km.

ColumnAmountSO2_TRU data are intended for studies on explosive volcanic eruptions where SO_2 is injected into the upper troposphere. The standard deviation over background areas is < 0.1 DU at all latitudes for TRU data. The TRU data can be used for investigating SO_2 plumes from explosive eruptions in the upper troposphere, but will overestimate SO_2 VCDs if the SO_2 plume altitude is higher than ~13 km.

ColumnAmountSO2_STL data are intended for studies on explosive volcanic eruptions where SO_2 is injected directly into the lower stratosphere at 16-20 km. STL data will underestimate total SO_2 amounts for plumes at lower altitudes. The standard deviation over background areas is < 0.1 DU at all latitudes.

2.5 Updates in Version 1.2

A key requirement in the PCA-based SO_2 retrieval approach is that the PCs derived from the radiance data and subsequently used in spectral fitting represent only non SO_2 features. Since globally SO_2 signals are relatively weak over most areas most of the time, this requirement is met in the vast majority of situations. One rare but notable exception occurs when volcanic eruptions emit large amounts of SO_2 into the atmosphere. Strong absorption of UV radiation by SO_2 from these eruptions cause significant changes in the Earthshine radiances measured by the OMPS instrument. As a result, PCs derived from those radiance data often contain strong SO_2 related spectral features.

In NMSO2_PCA_L2 V1.1 product, we implemented a scheme to exclude these SO_2-contaminated PCs in spectral fitting by examining the correlation between the PCs and SO_2 cross sections. While this check is effective for a number of volcanic eruptions observed by OMPS during 2012-2019, we also note that retrievals for some particularly large eruptions can still be problematic (see Figure 1a for an example).

In V1.2, we have added a new volcanic SO_2 flagging scheme to detect OMPS pixels with substantial volcanic SO_2 signals. This scheme is based on the differences in ozone retrieval residuals from two wavelength pairs (313 and 314 nm, and 314 and 315 nm). The residuals represent the differences between the measured and calculated radiances at different wavelengths in an ozone retrieval that assumes little or no SO_2 in the atmosphere. Under most conditions, this is a valid assumption and the residuals are similar between, for example, 313 and 314 nm. In the presence of large amounts of SO_2 from volcanic eruptions, however, the residuals are much greater at 313 nm than at 314 nm, as SO_2 absorbs much more strongly at the former wavelength. Tests with OMPS data have shown that the scheme can effectively detect pixels with ~5 DU of SO_2 in the stratosphere.

In NMSO2_PCA_L2 V1.2 product, this new volcanic SO_2 flagging scheme is run first and the OMPS pixels flagged by the scheme are excluded from the PCA analysis. This helps to minimize the impacts of large volcanic eruptions and significantly improves retrievals in those situations (see Figure 1b).

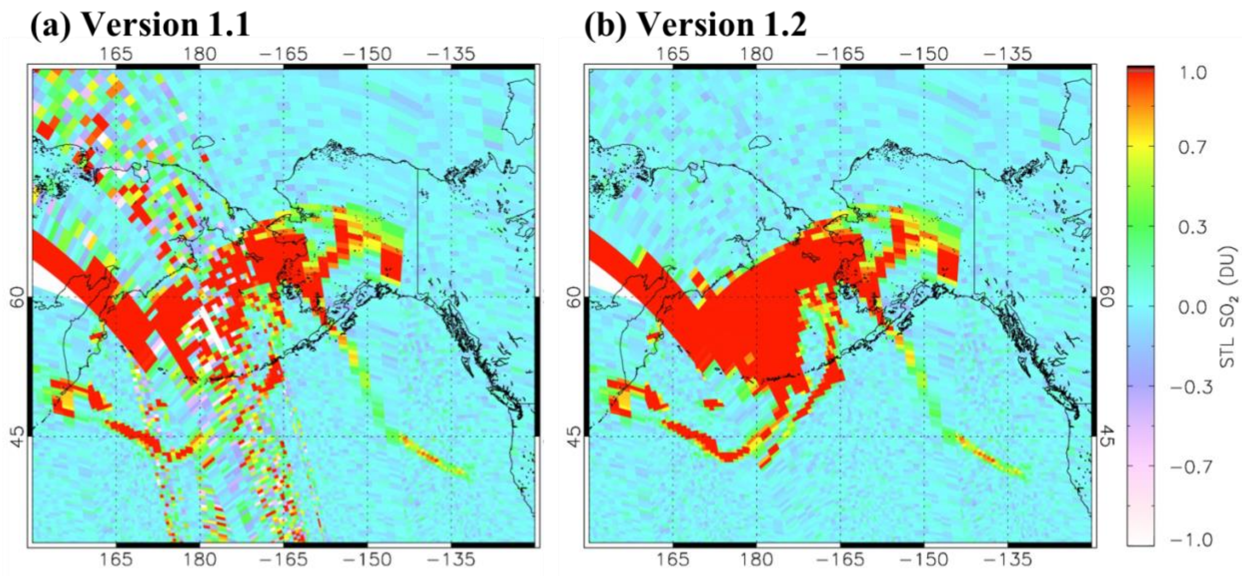

Figure 1. The volcanic SO_2 flagging scheme implemented in NMSO2_PCA_L2 V1.2 significantly improves retrieval quality for some large eruptions. The example in the figure shows STL (18-km *a priori* profile) SO_2 retrievals for the Raikoke plume on June 24, 2019 in (a) V1.1 and (b) V1.2 of the NMSO2_PCA_L2 product.

2.6 Updates in Version 2.0

In NMSO2_PCA_L2 V2.0, three estimates of SO_2 abundance are provided for air quality applications (also see section 3.3).

SlantColumnAmountSO2 (SCD) dataset contains the slant column densities (SCDs) of SO_2 and can be converted to VCDs using air mass factors (AMFs). For data users who wish to continue to use the previous ColumnAmountSO2_PBL dataset in NMSO2_PCA_L2 V1.2 and earlier, we recommend that a fixed AMF of 0.36 be used to convert the SCDs to VCDs, which in turn can be used as a continuity dataset in place of the original ColumnAmountSO2_PBL.

For most applications and studies related to anthropogenic SO_2 pollution, we recommend the use of ColumnAmountSO2, a new dataset of SO_2 VCDs in NMSO2_PCA_L2 V2.0 retrieved using updated Jacobian lookup tables and more realistic monthly *a priori* profiles based on model simulations.

The updated ColumnAmountSO2_PBL in NMSO2_PCA_L2 V2.0 is significantly different from the original ColumnAmountSO2_PBL in NMSO2_PCA_L2 V1.2 and earlier. In V2.0 it is produced with SO_2 Jacobians using the same new lookup tables as in

ColumnAmountSO2, but different *a priori* profiles assuming well-mixed SO_2 below 1 km and negligible SO_2 above 1 km. The dataset is recommended for studies of large point sources of SO_2.

3. DATASET ORGANIZATION

The NMSO2_PCA_L2 product is a set of Level 2 orbital swath files that follow a specific file naming convention and dataset organization.

3.1 File Naming Convention

The NMSO2_PCA_L2 product files are named as in this example:

OMPS-NPP_NMSO2-PCA-L2_v2.0_2017m0601t171237_o29118_2017m1013t150510.h5

The components of the filename are as follows:

1. Instrument (OMPS)
2. Spacecraft (NPP)
3. Product Name (NMSO2-PCA-L2)
4. Product Version (2.0)
5. Date and Time at Start of Orbit (2017-06-01 17:12:37 UTC)
6. Orbit Number (29118)
7. Production Date and Time (2017-10-13 15:05:10 UTC)
8. File Type (h5)

3.2 File Format and Structure

The NMSO2_PCA_L2 product files are in plain HDF5 that is netCDF4-compatible and CF-compliant. Each product file contains global attributes, dimensions, an ancillary data group, a geolocation data group, and a science data group.

3.3 Key Science Datasets

There are seven key science datasets in the SCIENCE_DATA group in each NMSO2_PCA_L2 product file. Six of these datasets correspond to the six estimates of the total vertical column densities (VCDs) of SO_2 assuming different *a priori* profiles. A seventh dataset contains the slant column densities (SCDs) of SO_2.

3.3.1 SlantColumnAmountSO2 (new in NMSO2_PCA_L2 V2.0)

Slant column densities (SCDs) of SO_2 produced by spectral fitting using SO_2 cross sections. When converted to VCDs with a fixed air mass factor (AMF) of 0.36, this newly introduced dataset in NMSO2_PCA_L2 V2.0 can be used as a continuity product for our previous Planetary Boundary Layer (PBL) SO_2 VCDs (ColumnAmountSO2_PBL) in NMSO2 V1.2 and earlier.

3.3.2 ColumnAmountSO2 (new in NMSO2_PCA_L2 V2.0)

ColumnAmountSO2 contains the vertical column densities (VCDs) of SO_2 produced by spectral fitting using updated SO_2 Jacobians that more accurately account for the effects of geometry, clouds, O_3, and surface reflectivity on OMPS sensitivity as well as updated *a priori* profiles from model simulations. This new dataset introduced in NMSO2_PCA_L2 V2.0 is recommended for most studies on air quality.

3.3.3 ColumnAmountSO2_PBL (updated in NMSO2_PCA_L2 V2.0)

SO_2 VCDs based on the same lookup tables as ColumnAmoutnSO2, but different *a priori* profiles assuming fixed mixing ratio within the lowest 1 km of the atmosphere and negligible SO_2 above. The ColumnAmountSO2_PBL dataset is recommended for use in studies on SO_2 emission sources. Note that ColumnAmountSO2_PBL in NMSO2_PCA_L2 V2.0 differs from the original ColumnAmountSO2_PBL dataset in NMSO2_PCA_L2 V1.2 and earlier.

3.3.4 ColumnAmountSO2_TRL

ColumnAmountSO2_TRL contains the estimated total VCDs of SO_2 in DU assuming a center of mass altitude of 3 km.

3.3.5 ColumnAmountSO2_TRM

ColumnAmountSO2_TRM contains the estimated total VCDs of SO_2 in DU assuming a center of mass altitude of 8 km.

3.3.6 ColumnAmountSO2_TRU

ColumnAmountSO2_TRU contains the estimated total VCDs of SO_2 in DU assuming a center of mass altitude of 13 km.

3.3.7 ColumnAmountSO2_STL

ColumnAmountSO2_STL contains the estimated total VCDs of SO_2 in DU assuming a center of mass altitude of 18 km.

4. FILE FORMAT

This section describes the file format of the Version 2.0 OMPS_NPP_NMSO2_PCA_L2 product, including the file-level attributes, dimensions, groups, variable-level attributes, fill values, geolocation data variables, ancillary data variables, and science data variables.

4.1 File-Level Attributes

The following table describes the 42 file-level attributes that appear at root level in the OMPS_NPP_NMSO2_PCA_L2 product.

Attribute Name	Description	Data Type
AuthorAffiliation	The institutional affiliation of the author(s).	string
AuthorName	The name(s) of the author(s).	string
Conventions	The conventions plus version numbers used in the product.	string
DataSetQuality	An assessment of the quality of the data.	string
DayNightFlag	The flag indicating whether the observations were made on the day or night side of Earth.	string
EastBoundingCoordinate	The longitude of the easternmost data in the granule.	32-bit floating-point
EquatorCrossingDate	The date of the ascending equator crossing of the orbit.	string
EquatorCrossingLongitude	The longitude of the ascending equator crossing of the orbit.	32-bit floating-point
EquatorCrossingTime	The time of the ascending equator	string

	crossing of the orbit.	
FOVResolution	The highest resolution on the ground of the observations.	string
GranuleDay	The day of the month at the beginning of the granule.	32-bit integer
GranuleDayOfYear	The day of the year at the beginning of the granule.	32-bit integer
GranuleMonth	The month of the year at the beginning of the granule.	32-bit integer
GranuleYear	The year at the beginning of the granule.	32-bit integer
HDFVersion	The version of HDF used to produce the granule.	string
InputPointer	A list of the input file(s) used to produce the granule.	string
InstrumentShortName	The short name of the instrument.	string
LocalGranuleID	The full name of the granule.	string
LocalityValue	The flag indicating the locality of the granule.	string
LongName	The long name of the product.	string
NorthBoundingCoordinate	The latitude of the northernmost data in the granule.	32-bit floating-point
NumberOfTimes	The number of lines of observations in the granule.	32-bit integer
OrbitNumber	The orbit number of the granule.	32-bit integer
PGEVersion	The version of the software that produced the granule.	string
ParameterName	The name of the geophysical parameter contained in the product.	string
PlatformShortName	The short name of the platform carrying the instrument.	string
ProcessLevel	The processing level of the granule.	string
ProcessingCenter	The data processing facility that produced the granule.	string
ProductType	The type of product.	string
ProductionDateTime	The production date-time of the granule.	string
RangeBeginningDate	The date at the beginning of the granule.	string
RangeBeginningTime	The time at the beginning of the granule.	string
RangeEndingDate	The date at the end of the granule.	string

RangeEndingTime	The time at the end of the granule.	string
SensorShortName	The short name of the sensor.	string
ShortName	The short name of the product.	string
Source	The platform and instrument that gathered the observations for the product.	string
SouthBoundingCoordinate	The longitude of the southernmost data in the granule.	32-bit floating-point
VersionID	The product version.	string
WestBoundingCoordinate	The longitude of the westernmost data in the granule.	32-bit floating-point
identifier_product_doi	The Digital Object Identifier (DOI) of the product.	string
identifier_product_doi_authority	The URL of the relevant DOI authority.	string

4.2 Dimensions

The following table describes the six dimensions in the OMPS_NPP_NMSO2_PCA_L2 product.

Dimension Name	**Description**	**Dimension Size**
nCorners	The dimension representing the corner number (1-based) of the ground pixel.	4
nLayers	The dimension representing the layer number (1-based) of the *a priori* profile.	72
nTimes	The dimension representing the along-track line number (1-based) in the granule.	varies from granule to granule
nWavel2	The dimension representing the wavelength index for the fitting windows.	2
nWavel3	The dimension representing the wavelength index for dNdR and SLER.	3
nXtrack	The dimension representing the cross-track position number (1-based) of the observation in the line.	36

4.3 Groups

The following table describes the three groups attached at root level in the OMPS_NPP_NMSO2_PCA_L2 product.

Group Name	Description
GEOLOCATION_DATA	Contains the 13 geolocation data variables.
ANCILLARY_DATA	Contains the two ancillary data variables.
SCIENCE_DATA	Contains the 29 science data variables.

4.4 Variable-Level Attributes

The following table describes the attributes attached to the variables in the OMPS_NPP_NMSO2_PCA_L2 product. Not all attributes are applicable to every variable.

Attribute Name	Description	Data Type
_FillValue	The fill value used for the variable.	same as for variable
bounds	The path to the relevant ground-pixel-corner coordinates variable (applies to the Latitude and Longitude variables only).	string
coordinates	The paths to the relevant coordinate variables (if applicable).	string
description	A detailed description of the variable.	string
long_name	The name for the variable that can be used in plots.	string
standard_name	The standard name for the variable (if applicable).	string
units	The units for the variable.	string
valid_max	The maximum valid value for the variable.	same as for variable
valid_min	The minimum valid value for the variable.	same as for variable

4.5 Fill Values

The following table summarizes the fill values used in the OMPS_NPP_NMSO2_PCA_L2 product.

Variable Data Type	Fill Value
32-bit integer	-2147483648
32-bit floating-point	-1.2676506E30
64-bit floating-point	-1.2676506002282294E30

4.6 Geolocation Variables

The following table describes the 13 geolocation variables in the OMPS_NPP_NMSO2_PCA_L2 product. The dimensions of these variables are nTimes for the 1-D variables (SpacecraftAltitude, SpacecraftLatitude, SpacecarftLongitude, Time and UTC_CCSDS_A), nTimes x nXtrack for the 2-D variables (Latitude, Longitude, SolarAzimuthAngle, SolarZenithAngle, ViewingAzimuthAngle and ViewingZenithAngle), and nTimes x nTrack x nCorners for the 3-D variables (LatitudeCorner and LongitudeCorner).

Variable Name	**Description**	**Data Type**
Latitude	The terrestrial latitude (in degrees) at the center of the ground pixel.	32-bit floating-point
LatitudeCorner	The terrestrial latitudes (in degrees) at the corners of the ground pixel.	32-bit floating-point
Longitude	The terrestrial longitude (in degrees) at the center of the ground pixel.	32-bit floating-point
LongitudeCorner	The terrestrial longitudes (in degrees) at the corners of the ground pixel.	32-bit floating-point
SolarAzimuthAngle	The solar azimuth angle (in degrees) at the center of the ground pixel.	32-bit floating-point
SolarZenithAngle	The solar zenith angle (in degrees) at the center of the ground pixel.	32-bit floating-point
SpacecraftAltitude	The altitude of the spacecraft (in m) at the time of observation.	32-bit floating-point
SpacecraftLatitude	The latitude of the spacecraft (in degrees) at the time of observation.	32-bit floating-point
SpacecraftLongitude	The longitude of the spacecraft (in degrees) at the time of observation.	32-bit floating-point
Time	TAI93 (in continuous seconds since 12 a.m. UTC on January 1, 1993) of the observation.	64-bit floating-point
UTC_CCSDS_A	UTC (in CCSDS ASCII Time Code a format) of the observation.	27-character string
ViewingAzimuthAngle	The viewing azimuth angle (in degrees) at the center of the ground pixel.	32-bit floating-point
ViewingZenithAngle	The viewing zenith angle (in degrees) at the center of the ground pixel.	32-bit floating-point

4.7 Ancillary Variables

The following table describes the two ancillary variables in the OMPS_NPP_NMSO2_PCA_L2 product. The dimensions for both variables are nTimes x nXtrack.

Variable Name	**Description**	**Data Type**
CloudPressure	The optical centroid pressure (in hPa) of the mixed LER model associated with the ground pixel (from NMCLDRR-L2).	32-bit floating-point
TerrainPressure	The terrain pressure (in hPa) at the center of the ground pixel (from NMTO3-L2).	32-bit integer

4.8 Science Variables

The following table describes the 29 science variables in the OMPS_NPP_NMSO2_PCA_L2 product. The dimensions for most of these variables are nTimes x nXtrack. LayerBottomPressure has dimension nLayers. FittingWindow_STL, FittingWindow_TRL, FittingWindow_TRM and Fitting_Window_TRU have dimensions nTimes x nTrack x nWavel2. SLER, Wavelength_SLER and dNdR have dimensions nTimes x nXtrack x nWavel3. GEOS5LayerWeight, PBLLayerWeight and ScatteringWeight have dimensions nTimes x nXtrack x nLayers.

Variable Name	**Description**	**Data Type**
AlgorithmFlag_SnowIce	The snow-ice algorithm flag associated with the ground pixel: 0 – no snow/ice, 1 – snow/ice covered and cloud free, 2 – possible snow/ice covered and cloud free, 3 – snow/ice covered and likely cloud covered.	32-bit integer
CloudFraction	The effective cloud fraction of the mixed LER model associated with the ground pixel (from NMCLDRR-L2).	32-bit floating-point
CloudRadianceFraction	The cloud radiance fraction at 313 nm associated with the ground pixel.	32-bit floating-point
ColumnAmountO3	The best total ozone solution (in DU) associated with the ground pixel (from NMTO3-L2).	32-bit floating-point

ColumnAmountSO2	The total vertical column amount SO_2 (in DU) associated with the ground pixel retrieved using a monthly mean *a priori* SO_2 profile from GEOS-5 model simulations.	32-bit floating-point
ColumnAmountSO2_PBL	The total vertical column amount SO_2 (in DU) associated with the ground pixel retrieved using a prescribed PBL SO_2 profile assuming constant mixing ratio within 1 km of the surface and negligible SO_2 above 1 km.	32-bit floating-point
ColumnAmountSO2_STL	The total vertical column amount SO_2 (in DU) associated with the ground pixel retrieved using a prescribed SO_2 profile centered at 18 km.	32-bit floating-point
ColumnAmountSO2_TRL	The total vertical column amount SO_2 (in DU) associated with the ground pixel retrieved using a prescribed SO_2 profile centered at 3 km.	32-bit floating-point
ColumnAmountSO2_TRM	The total vertical column amount SO_2 (in DU) associated with the ground pixel retrieved using a prescribed SO_2 profile centered at 8 km.	32-bit floating-point
ColumnAmountSO2_TRU	The total vertical column amount SO_2 (in DU) associated with the ground pixel retrieved using a prescribed SO_2 profile centered at 13 km.	32-bit floating-point
FittingWindow_STL	The fitting window (in nm) for the SO_2 STL retrieval.	32-bit floating-point
FittingWindow_TRL	The fitting window (in nm) for the SO_2 TRL retrieval.	32-bit floating-point
FittingWindow_TRM	The fitting window (in nm) for the SO_2 TRM retrieval.	32-bit floating-point
FittingWindow_TRU	The fitting window (in nm) for the SO_2 TRU retrieval.	32-bit floating-point
Flag_SAA	The South Atlantic Anomaly (SAA) flag associated with the ground pixel: 0 – not affected by SAA, 1 – affected by SAA.	32-bit integer
Flag_SO2	The SO_2 flag associated with the ground pixel: 0 – no detection of SO_2, 1 – potential SO_2 contamination.	32-bit integer
GEOS5LayerWeight	The *a priori* SO_2 profile associated with the ground pixel based on GEOS-5 model simulations, with the layer weight being the	32-bit floating-point

	fraction of SO_2 molecules contributed by each of the 72 vertical layers to the overall SO_2 molecules within the entire atmospheric column. The 72 vertical layers are defined by LayerBottomPressure and a top of the atmosphere pressure of 0.01 hPa.	
LayerBottomPressure	The pressure at the bottom of each of the 72 vertical layers for which the scattering weight and the *a priori* SO_2 profile are provided.	32-bit floating-point
PBLLayerWeight	The *a priori* SO_2 profile associated with the ground pixel assuming a fixed mixing ratio within 1 km of the surface and negligible SO_2 above 1 km. The layer weight represents the fraction of SO_2 molecules contributed by each of the 72 vertical layers to the overall SO_2 molecules within the entire atmospheric column. The 72 vertical layers are defined by LayerBottomPressure and a top of the atmosphere pressure of 0.01 hPa.	32-bit floating-point
Reflectivity342	The Simple Lambertian Equivalent Reflectivity (SLER) at 342 nm associated with the ground pixel.	32-bit floating-point
SLER	The Simple Lambertian Equivalent Reflectivity (SLER) associated with the ground pixel.	32-bit floating-point
ScatteringWeight	The scattering weight at 313 nm associated with the ground pixel for each of the 72 vertical layers as defined by LayerBottomPressure and a top of the atmosphere pressure of 0.01 hPa.	32-bit floating-point
SceneReflectivity354	The scene reflectivity at 354 nm associated with the ground pixel (from NMCLDRR-L2).	32-bit floating-point
SlantColumnAmountSO2	The retrieved slant column amount SO_2 (in molec/cm2) associated with the ground pixel.	32-bit floating-point
SurfaceReflectivity	The surface reflectivity at 360 nm associated with the ground pixel (from NMCLDRR-L2).	32-bit floating-point
UVAerosolIndex	The UV aerosol index (342.5 and 367 nm) associated with the ground pixel.	32-bit floating-point
Wavelengths_SLER	The wavelength (in nm) for the Simple Lambertian Equivalent Reflectivity (SLER)	32-bit floating-point

	associated with the ground pixel.	
dNdR	The reflectivity sensitivity ratio, dNdR, for the retrieval.	32-bit floating-point
nPrincipalComponents	The number of principal components for the retrieval.	32-bit integer

5. CONTACTS

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6. REFERENCES

Eisinger, M. and Burrows, J. P.: Tropospheric sulfur dioxide observed by the ERS-2 GOME instrument, *Geophys. Res. Lett.*, 25(22), 4177–4180, doi:10.1029/1998GL900128, 1998.

Fisher, B. L., Krotkov, N. A., Bhartia, P. K., Li, C., Carn, S. A., Hughes, E., and Leonard, P. J. T.: A new discrete wavelength backscattered ultraviolet algorithm for consistent volcanic SO_2 retrievals from multiple satellite missions, *Atmos. Meas. Tech.*, 12, 5137–5153, https://doi.org/10.5194/amt-12-5137-2019, 2019.

Flynn, L., Long, C., Wu, X., Evans, R., Beck, C. T., Petropavlovskikh, I., McConville, G., Yu, W., Zhang, Z., Niu, J., Beach, E., Hao, Y., Pan, C., Sen, B., Novicki, M., Zhou, S., and Seftor, C.: Performance of the Ozone Mapping and Profiler Suite (OMPS) products, *J. Geophys. Res.-Atmos.*, 119, 6181– 6195, doi:10.1002/2013JD020467, 2014.

Krotkov, N. A., Cam, S. A., Krueger, A. J., Bhartia, P. K. and Yang, K.: Band residual difference algorithm for retrieval of SO_2 from the Aura Ozone Monitoring Instrument (OMI), *IEEE Trans. Geosci. Remote Sens.*, 44(5), 1259–1266, doi:10.1109/TGRS.2005.861932, 2006.

Krueger, A. J., Sighting of El Chichón sulfur dioxide clouds with the Nimbus 7 Total Ozone Mapping Spectrometer, *Science*, 220, 1377–1378, 1983.

Labow, G. J., Ziemke, J. R., McPeters, R. D., Haffner, D. P., and Bhartia, P. K.: A total ozone-dependent ozone profile climatology based on ozone sondes and Aura MLS data, *J. Geophys. Res. Atmos.*,120, 2537–2545, doi:10.1002/2014JD022634, 2015.

Li, C., Joiner, J., Krotkov, N. A., and Bhartia, P. K.: A fast and sensitive new satellite SO_2 retrieval algorithm based on principal component analysis: Application to the ozone monitoring instrument, *Geophys. Res. Lett.*, 40, 6314–6318, doi:10.1002/2013GL058134, 2013.

Li, C., Krotkov, N. A., Carn, S., Zhang, Y., Spurr, R. J. D., and Joiner, J.: New-generation NASA Aura Ozone Monitoring Instrument (OMI) volcanic SO_2 dataset: Algorithm description, initial results, and continuation with the Suomi-NPP Ozone Mapping and Profiler Suite (OMPS), *Atmos. Meas. Tech.*, 10, 445–458, doi:10.5194/amt-10-445-2017, 2017.

Li, C., Krotkov, N. A., Leonard, P. J. T., Carn, S., Joiner, J., Spurr, R. J. D., and Vasilkov, A.: Version 2 Ozone Monitoring Instrument SO_2 product (OMSO2 V2): New anthropogenic SO_2 vertical column density dataset, *Atmos. Meas. Tech.*, under review, 2020.

Seftor, C. J., Jaross, G., Kowitt, M., Haken, M., Li, J., and Flynn, L. E.: Postlaunch performance of the Suomi National Polar-orbiting Partnership Ozone Mapping and Profiler Suite (OMPS) nadir sensors, *J. Geophys. Res.-Atmos.*, 119, 4413– 4428, doi:10.1002/2013JD020472, 2014.

Spurr, R.: LIDORT and VLIDORT: Linearized Pseudo-Spherical Scalar and Vector Discrete Ordinate Radiative Transfer Models for use in Remote Sensing Retrieval Problems, Light Scattering Reviews, vol. 3, edited by A. Kokhanovsky, Springer, Berlin Heidelberg, doi:10.1007/ 978-3-540-48546-9, 2008.

Vasilkov, A., Joiner, J., and Seftor, C.: First results from a rotational Raman scattering cloud algorithm applied to the Suomi National Polar-orbiting Partnership (NPP) Ozone Mapping and Profiler Suite (OMPS) Nadir Mapper, *Atmos. Meas. Tech.*, 7, 2897–2906, https://doi.org/10.5194/amt-7-2897-2014, 2014.

Yang, K., Krotkov, N., Krueger, A., Carn, S., Bhartia, P., and Levelt, P.: Retrieval of large volcanic SO_2 columns from the Aura Ozone Monitoring Instrument: Comparison and limitations, *J. Geophys. Res.*, 112, D24S43, doi:10.1029/2007JD008825, 2007.

Zhang, Y., Li, C., Krotkov, N. A., Joiner, J., Fioletov, V. and McLinden, C.: Continuation of long-term global SO_2 pollution monitoring from OMI to OMPS, *Atmos. Meas. Tech.*, 10, 1495–1509, doi:10.5194/amt-10-1495-2017, 2017.