Overview

This document describes the OMI SO_2 product (OMSO2) produced from global mode UV measurements of the Ozone Monitoring Instrument (OMI). OMI was launched on July 15, 2004 on the EOS Aura satellite, which is in a sun-synchronous ascending polar orbit with 1:45 pm local equator crossing time. The data collection started on August 17, 2004 (orbit 482) and continues to this day with only minor data gaps. The minimal volcanic SO_2 mass detectable by OMI is about two orders of magnitude smaller than the detection threshold of the legacy Total Ozone Mapping Spectrometer (TOMS) SO_2 data (1978-2005) [Krueger et al 1995]. OMI also enables the detection of anthropogenic SO_2 pollution in the lowest part of the atmosphere. This is due to smaller OMI footprint and the use of wavelengths better optimized for separating O_3 from SO_2.

The product file, called a data granule, covers the sunlit portion of the orbit with an approximately 2600 km wide swath. Each swath normally contains approximately 1600 viewing lines along the ground track of the satellite, with each viewing line containing 60 pixels or scenes across the satellite track. Scenes from all viewing lines with the same cross-track scene number are referred to as a row of the OMI swath. During normal operations, 14 or 15 granules are produced daily, providing fully contiguous coverage of the globe. Currently, OMSO2 products are not produced when OMI goes into the "zoom mode" for one day every 452 orbits.

Since 25 June 2007 signal suppression (anomaly) has been observed in Level 1B Earth radiance data for scenes in rows 53-54 (0-based). This anomaly is also known as the OMI row anomaly since it affects some particular rows of the CCD detector. It has since expanded to affect more rows. In SO_2 data, the row anomaly manifests itself as positive or negative stripes (discontinuity in SO_2 with cross-track viewing angle). Efforts have been made to flag the affected scenes. SO_2 data fields for scenes determined to have been influenced by the row anomaly have been assigned a large negative fill-value. More information about the OMI row anomaly can be found from KNMI.

For each OMI scene we provide 4 different estimates of the vertical column density of SO_2 in Dobson Units (1 DU = $2.69 \cdot 10^{16}$ molecules/cm^2) obtained by making different assumptions about the vertical distribution of the SO_2. However, it is important to note that in most cases the precise vertical distribution of SO_2 is unimportant. The users can use either the SO_2 plume height, or the center of mass altitude (CMA) derived from SO_2 vertical distribution, to interpolate between the 4 values:

- Planetary Boundary Layer (PBL) SO_2 column (**ColumnAmountSO2_PBL**), corresponding to CMA of 0.9 km, recommend for use in studies on near-surface pollution. **Please check the following section for important updates to the PBL SO_2 data in OMSO2 product version 1.2 and later.**

- Lower tropospheric SO_2 column (**ColumnAmountSO2_TRL**) corresponding to CMA of 3 km, recommended for use in studies on degassing from volcanic sources. **Please check the section following the next section for important**

updates to the TRL, TRM, and STL SO_2 data in OMSO2 product version 1.3.

- Middle tropospheric SO_2 column (**ColumnAmountSO2_TRM)** corresponding to CMA of 8 km, recommended for use in studies on moderate eruptions and long-range transport of sulfur pollution,

- Lower stratospheric SO_2 column (**ColumnAmountSO2_STL**) corresponding to CMA of 18 km, recommended for use in studies on explosive volcanic eruptions.

The accuracy and precision of the derived SO_2 columns vary significantly with the SO_2 CMA and column amount, observational geometry, and slant column ozone. OMI becomes more sensitive to SO_2 above clouds and snow/ice, and less sensitive to SO_2 below clouds. Preliminary error estimates are discussed below (see Data Quality Assessment).

Important Updates to OMI PBL SO_2 Data (Version 1.2 and later)

The SO_2 data in **ColumnAmountSO2_PBL** are now produced with a retrieval algorithm based on principal component analysis (PCA) of the OMI radiance data [Li et al 2013]. Previously the OMI PBL SO_2 data were produced using the Band Residual Difference (BRD) algorithm [Krotkov et al 2006]. While the BRD algorithm is sensitive to SO_2 pollution in the PBL, it tends to have large noise and unphysical biases particularly at high latitudes. The PCA algorithm greatly improves the quality of OMI SO_2 retrievals and has been implemented for operational production of the next generation OMI standard SO_2 product. **In OMSO2 product version 1.2 or later, the entire PBL SO_2 data record has been reprocessed with the PCA algorithm. PBL SO_2 Users who had previously acquired the old version OMSO2 data before the data release in October 2014 are strongly encouraged to download and use the new OMSO2 product (version 1.2 or later). There is no difference in the PBL SO_2 between version 1.2 and version 1.3 of the OMSO2 product. All SO_2 data fields ending with "BRD" are obsolete and only used for internal diagnostic purposes.**

Important Updates to Version 1.3 OMI Volcanic (TRL, TRM, STL) SO_2 Data

The SO_2 data in **ColumnAmountSO2_TRL, ColumnAmountSO2_TRM, and ColumnAmountSO2_STL data fields in the version 1.3 OMSO2 product** are now produced with an extended version of the PCA algorithm [Li et al 2016]. Previously the OMI TRL, TRM, and STL SO_2 data were produced using the linear fit (LF) algorithm [Yang et al 2007]. While the LF algorithm is fast and sensitive to SO_2 from volcanic eruptions, it has a tendency to underestimate large volcanic SO_2 signals due to saturation of SO_2 absorptions at the strongly absorbing short UV wavelengths (< 315 nm). It also has relatively large noise and artifacts as compared with the PCA algorithm. **The entire**

OMI TRL, TRM, and STL SO_2 datasets in the OMSO2 product have been reprocessed with the new PCA-based algorithm. Volcanic (TRL, TRM, and STL) SO_2 data users who had previously acquired OMSO2 data prior to the data release in June 2016 are strongly encouraged to download and use the new version 1.3 OMSO2 product.

Algorithm Description

All OMI SO_2 data are now generated with principal component analysis (PCA) -based algorithms. The PBL columns in OMSO2 version 1.2 and later are produced using the original PCA algorithm with a fixed spectral fitting window and a fixed SO_2 Jacobian spectrum that are appropriate for pollution SO_2 near the surface [Li et al 2013]. There is no difference in the PBL SO_2 between version 1.2 and version 1.3 of the OMSO2 product. TRL, TRM, and STL SO_2 columns in the new OMSO2 version 1.3 are produced with an extended version of the PCA algorithm, using a spectral fitting window and SO_2 Jacobians lookup table (LUT) suitable for volcanic SO_2 signals [Li et al 2016].

In the PBL SO_2 PCA algorithm, we apply a principal component analysis technique to radiance data over a presumably SO_2-free region (*e.g.*, the equatorial Pacific). The resulting principal components (PCs) can capture most (> 99.9999%) of measurement-to-measurement variation of the radiances. The PCs are ordered so that the first PC explains the most of spectral variance, the second PC explains the second most of spectral variance, and so on. The first few leading PCs are generally associated with geophysical processes including ozone absorption, surface reflectance, and rotational-Raman scattering effects (RRS, also known as the Ring effect), while the following PCs often have high-frequency features likely originating from measurement noise and detector artifacts such as wavelength shift and stretch. These physical processes and measurement details can cause strong interferences in SO_2 retrievals, and the PCs enable us to appropriately account for them. By fitting a set of n_v PCs (v_i) along with the SO_2 Jacobians, which represents the sensitivity of the radiances to the SO_2 column ($\partial N/\partial\Omega_{SO_2}$), to the measured Sun-normalized radiances, we can simultaneously obtain estimates of SO_2 column density (Ω_{SO2}) and coefficients of the PCs ($\boldsymbol{\omega}$):

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

Here N is the measured N-value spectrum ($N(\lambda) = -100\times\log_{10}(I(\lambda)/I_0(\lambda)$, I and I_0 are radiance and irradiance at wavelength λ, respectively) for a given OMI scene. The PCA algorithm shares the same overall physics concept with the widely used Differential Optical Absorption Spectroscopy (DOAS) method, but the data-driven (vs. forward modeling) approach used to account for retrieval interferences reduces modeling uncertainties, enhances computation efficiency, and makes the PCA algorithm much less sensitive to instrument calibration issues. A more detailed discussion of the PCA algorithm can be found in Li et al [2013] and Joiner et al [2013].

For input data, the PCA algorithm uses OMI level 1B (L1B) radiance and irradiance data in the spectral window of 310.5-340 nm, as well as the O_3 column amount (Ω_{O3}) from the OMTO3 product [Bhartia and Wellemeyer 2002]. The spectral window includes the strong SO_2 absorption band at 310.8 nm and minimizes potential interferences due to stray light at shorter wavelengths. To better account for the orbit-to-orbit measurement artifacts and the different characteristics of the 60 rows of the OMI detector, we process data from each row of each orbit separately. Scenes having strong O_3 absorption due to large slant column O_3 (S_{O3} > 1500 DU) are filtered out before PCA, given the much smaller expected SO_2 sensitivity for these scenes. After data filtering, we first conduct PCA on the approximately 900-1300 remaining scenes for an entire row, without screening out polluted areas. Since SO_2 absorption is generally very weak outside of polluted and volcanic-affected areas, it is unlikely for the PC(s) associated with or affected by SO_2 absorption (v_{so2}) to be among the first few leading PCs. A correlation analysis between the PCs and the SO_2 Jacobians is then conducted to determine the number of PCs (n_v) to be included in the fitting. This ensures that n_v is sufficiently small to prevent the inclusion of v_{so2} and collinearity in Eq. 1, and allows reasonable initial estimates of SO_2 (Ω_{SO2_ini}) to be obtained. To maintain computational efficiency, we set an upper limit of 20 for n_v. A second step PCA is then applied to scenes with small Ω_{SO2_ini} (within ±1.5 standard deviations for each orbit/row) to extract a new set of PCs to update Eq. 1, followed by updated retrievals of SO_2. This step is repeated twice, as the changes in the retrieved SO_2 generally become very small within two iterations. The second step PCA and retrievals are carried out separately for three segments of each row: a "tropical" region with S_{O3} < 100 DU + min(S_{O3}), and two regions north and south of it. These regionally derived PCs more closely match the measurements and help reduce retrieval biases.

The SO_2 Jacobians used in the current version of the PBL SO_2 PCA algorithm are calculated with the VLIDORT radiative transfer code [Spurr 2008]. The calculation assumes the same measurement conditions as those in the BRD algorithm. More specifically, we assume fixed surface albedo (0.05), surface pressure (1013.25 hPa), as well as fixed solar zenith angle (30°) and viewing zenith angle (0°). For SO_2, a climatological profile over the summertime eastern U.S. are used. For O_3 and temperature, the OMTO3 standard mid-latitude profiles with Ω_{O3} = 325 DU are used. This setup allows direct comparison between the new and old OMI PBL SO_2 data. In the future, we plan to expand the look-up table for SO_2 Jacobians to more realistically account for different measurement conditions.

New for version 1.3 OMSO2 data: the PCA-based volcanic (TRL, TRM, and STL) SO_2 retrieval algorithm [Li et al 2016] is an extended version of the PBL SO_2 PCA algorithm. The algorithm consists of two parts. The first part is essentially identical to the PBL SO_2 algorithm as described above and is used to provide input to the second part of the algorithm, including initial estimates of SO_2 column amounts (Ω_{SO2_ini}) and principal components (PCs) to be used in spectral fitting. The second part of the algorithm produces more accurate estimates of volcanic SO_2 column amounts by conducting iterative spectral fitting and by using a more comprehensive lookup table for SO_2 Jacobians. We followed an approach similar to that in TOMS and OMI total column O_3

retrievals [Bhartia and Wellemeyer 2002], and used simple Lambertian equivalent reflectivity (SLER or *R*) derived at the surface [Ahmad et al 2004] to implicitly account for the combined effects of aerosols, clouds, and the surface on the spectral dependence of TOA (top of the atmosphere) radiances and SO_2 Jacobians. We also neglected the effects of non-elastic rotational Raman scattering (RRS) on SO_2 Jacobians. As a result, the backscattered radiances at TOA (*I*) for multiple elastic Rayleigh scattering can be calculated with the following equation:

$$I = I_0(\theta_0, \theta) + I_1(\theta_0, \theta)\cos\phi + I_2(\theta_0, \theta)\cos 2\phi + \frac{R I_r(\theta_0, \theta)}{(1 - R S_b)}. \qquad (2)$$

The first three terms (I_0, I_1, and I_2) on the right-hand side (RHS) of the equation represent the atmospheric component the back-scattered radiances, while the last term represents the surface component. θ_0, θ, and ϕ stand for solar zenith angle (SZA), viewing zenith angle (VZA), and relative azimuth angle (RAZ), respectively. Taking the partial derivative with respect to Ω_{SO2}, we obtained the following equation used for the determination of SO_2 Jacobians:

$$\frac{\partial I}{\partial \Omega_{so2}} = \frac{\partial I_0(\theta_0,\theta)}{\partial \Omega_{so2}} + \frac{\partial I_1(\theta_0,\theta)}{\partial \Omega_{so2}}\cos\phi + \frac{\partial I_2(\theta_0,\theta)}{\partial \Omega_{so2}}\cos 2\phi + \frac{R}{(1-RS_b)}\frac{\partial I_r(\theta_0,\theta)}{\partial \Omega_{so2}} + \frac{R^2 I_r(\theta_0,\theta)}{(1-RS_b)^2}\frac{\partial S_b}{\partial \Omega_{so2}}$$
(3)

Using VLIDORT, we built a set of pre-computed multi-dimensional SO_2 Jacobian lookup tables, with eight SZA nodes (0-81°), eight VZA nodes (0-80°), and 15 SO_2 nodes (0-1000 DU), for each of the 21 standard O_3 climatology profiles used in OMI total O_3 retrievals [Bhartia and Wellemeyer 2002]. This was done separately for four different prescribed SO_2 profiles (TRL, TRM, and STL) at 0.05 nm spectral resolution for the spectral range of 311-342 nm.

For a given pixel with SZA = θ_0, VZA = θ, RAZ = ϕ, initial estimate of SO_2 total column amount of Ω_{SO2_ini}, and O_3 column amount of Ω_{O3}, the algorithm first determines SLER (*R*) 342.5, 354.1, 367.04 nm, where contributions from gaseous absorption and non-elastic RRS processes are minimal, and then extrapolates *R* at these wavelengths to shorter wavelengths (310-340 nm). The algorithm then determines the SO_2 Jacobian spectrum for the pixel by interpolating Jacobians calculated using equation (3) for two O_3 (corresponding to two different O_3 climatology profiles), two SO_2, two SZA, and two VZA nodes that bracket Ω_{O3}, Ω_{SO2_ini}, θ_0, and θ, respectively. Details on how the SO_2 Jacobians are calculated are given in Li et al [2016].

The SO_2 Jacbobian spectrum and the principal components from the first part of the algorithm are fit to the measured radiances in the nominal fitting window of 313-340 nm to produce an updated estimate of SO_2 VCD (Ω_{SO2_step1}) for the pixel and compared with Ω_{SO2_ini}. If the difference is greater than 0.1 DU or 1% for pixels with SO_2 > 100 DU, Ω_{SO2_step1} is used as input to the lookup table to update the SO_2 Jacobian spectrum. The iterations continue until the results converge or the number of iterations exceeds 15. In each iteration step, the left edge of the actual fitting window is determined by locating the wavelength with the largest SO_2 Jacobian within 313-340 nm (up to 326.5 nm or roughly the mid-point of this nominal fitting window). All wavelengths shorter than this wavelength are excluded in the spectral fitting. This approach allows the interpolation error due to signal saturation at short UV wavelengths to be minimized.

Data Quality Assessment

Errors in OMI SO_2 data can arise from both the input radiance/residual data and the SO_2 Jacobians used in retrievals. The resulted errors are best described as pseudo-random (i.e. having different systematic and random components depending on spatial and temporal scales) Gaussian-like distribution with a nominal mean of zero. The errors usually reduce much slower than the square root of the number of measurements averaged.

We provide separate Quality Flags (QF) for each of the products that are based on SO_2 consistency criteria between the individual wavelength pairs. The OMSO2 scene quality flag is an automatic assessment of the SO_2 values for the corresponding scene by the OMSO2 retrieval algorithm. It is used primarily as an indicator of the validity of the retrieved SO_2 values. For detailed information about the OMSO2 quality flag, please consult the OMSO2 file specification). **While the quality flag may provide some information on the usefulness of retrievals, we have found it to be too restrictive and not very useful in its current form.** Preliminary analysis of the QF values has shown that they may miss many real PBL and low level degassing emissions. Therefore, independent verification of the real SO_2 signal is strongly recommended. **OMSO2 data users are advised to ignore the quality flag in the current version and use other parameters such as solar zenith angle for data filtering, as specified below for the PBL data and volcanic SO_2 data**. Below are data quality assessments for each SO_2 product. For all products the noise increases with increasing solar zenith angle at high latitudes and in the region of "South Atlantic radiation Anomaly".

ColumnAmountSO2_PBL: As a measurement of retrieval noise, the standard deviation (sigma) for instantaneous field of view (IFOV) is ~0.5 DU over the presumably SO_2-free equatorial Pacific for PBL SO_2 in OMSO2 product version 1.2 or later, or about half that of the BRD algorithm. The root mean square (RMS) for IFOV in different latitude bands over the Pacific can be viewed as a measure of both noise and biases in retrievals, and is estimated at ~0.5 DU for regions between 30°S and 30°N, suggesting very small systematic biases in PCA retrievals over the tropics. The IFOV RMS of PCA retrievals increases to ~0.7-0.9 DU for high latitude regions with large slant column O_3, but is still more than a factor of two smaller than that of BRD retrievals. **Data users are advised to use caution when analyzing data from the edges of the OMI swath (rows 0 and 59, 0-based), as they tend to have greater noise. For best data quality, use data from scenes near the center of the swath (rows 4-54, 0-based) with slant column O_3 < 1500 DU. Retrievals for OMI scenes from the descending node of the Aura satellite should not be used.** The PCA retrievals also have a negative bias over some highly reflective surfaces such as certain areas in the Sahara (up to about -0.5 DU in monthly mean). This negative bias is small as compared to the biases in the BRD retrievals, and is expected to be further reduced after the implementation of a more extensive Jacobians lookup table (see below). For cloudy scenes, the BRD algorithm sometimes produces large negative retrievals, a bias that is now eliminated in the PCA retrievals.

The SO_2 retrieval accuracy also depends on the error in the SO_2 Jacobians. This error is systematic and increases with deviation of the observational conditions from those assumed in the Jacobian calculation. SO_2 will likely be overestimated for remote oceanic regions where SO_2 is transported from source regions and likely located at elevated levels above the PBL. Likewise, SO_2 will also be overestimated for scenes with snow/ice and/or clouds. We plan to expand the look-up table for SO_2 Jacobians to more realistically account for different measurement conditions. **Before this improvement, only snow/ice-free scenes with radiative cloud fraction < 0.3 should be used in studies on SO_2 emission sources.** The higher reflectivity scenes can still be used to track long-range transport of sulfur pollution. Finally, there is also a small but noticeable dependence of retrieved SO_2 on the number of PCs included in the fitting. We expect to provide a more complete error estimate in follow-up releases.

New for version 1.3 OMSO2 data:
ColumnAmountSO2_TRL: Due to increased sensitivity to elevated SO_2, the pixel-level 1 sigma noise in TRL data is estimated at ~0.2 DU under optimal observational conditions in the tropics. The noise is about 0.3 DU for high latitudes. The data can be used for cloudy, clear and mixed scenes as well as for elevated terrain, but will overestimate SO_2 plumes at altitudes higher than 3 km. Since the noise level of the new PCA TRL SO_2 is about a factor of two smaller than the previous LF TRL SO_2, we now recommend that the TRL retrievals be used for estimating emissions from degassing volcanoes.

ColumnAmountSO2_TRM: The standard deviation of TRM retrievals in background areas is about 0.1 DU in the tropics and about 0.15 DU at high latitudes, again about a factor of two smaller than the previous LF TRM retrievals. 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.

ColumnAmountSO2_STL data are intended for use for explosive volcanic eruptions where SO_2 is injected into the upper troposphere or lower stratosphere (UTLS). The standard deviation over background areas is around 0.1 DU for all latitudes for STL data.

Unlike the LF algorithm that has large negative bias for high SO_2 loading cases (> 100 DU), the new PCA volcanic SO_2 algorithm has greatly reduced this error and compares well with other retrieval methods that also utilize the full spectral content of UV hyperspectral measurements. For example, for the Kasatochi eruption in August 2008, the PCA-estimated total SO_2 loading is ~1700 kt, about a factor of two higher than the estimate based on LF retrievals and generally in good agreement with the offline OMI iterative spectral fitting (ISF) retrievals and GOME-2 optimal estimation retrievals. For the Sierra Negra eruption in October 2005, the PCA algorithm yields a max SO_2 of over 1100 DU. This agrees well with the offline OMI ISF retrievals and is several times greater than the max SO_2 from the LF algorithm. It should be noted that the PCA algorithm might still underestimate SO_2 loading for highly concentrated plumes immediately after large eruptions. Additionally, some eruptions also emit large amounts of dust into the atmosphere that may interfere with SO_2 retrievals. This interference may not necessarily be appropriately accounted for using the SLER approach and may cause errors in the retrieved SO_2.

Volcanic SO_2 data from all rows of the OMI, with the exception of rows affected by the row anomaly, can be used. As with the PBL SO_2 data**, it is best to use retrievals from scenes with SZA < 70°, and retrievals for OMI scenes from the descending node of the Aura satellite should not be used.** When estimating the SO_2 loading from a volcanic plume within a given domain, it is recommended that only OMI scenes or pixels exceeding a certain threshold (e.g., 1 DU) be included in the calculation. This helps to filter out occasional negative retrieval noise.

Product Description

The OMSO2 product is written as HDF-EOS5 swath file. Data files are available from Goddard Earth sciences Data and Information Services Center (GES DISC) web site. For a list of tools that read HDF-EOS5 data files, please visit this link:
http://disc.gsfc.nasa.gov/Aura/tools.shtml

A file, also called a granule, contains SO_2 and associated information retrieved from each OMI scene from the sun-lit portion of an Aura orbit. The data are ordered in time sequence. The information provided on these files includes: latitude, longitude, solar zenith angle, OMTO3 reflectivity (LER) and independent estimates of the SO_2 vertical columns, as a well as a number of ancillary parameters that provide information to assess data quality. Four values of SO_2 column amounts are provided corresponding to four assumed vertical profiles. Independent information is needed to decide which value is most applicable. For a complete list of the parameters, please read the OMSO2 file Specification.

For general assistance with data archive, please contact GES DISC. For questions and comments related to the OMSO2 algorithm and data quality please contact Nickolay Krotkov (Nickolay.A.Krotkov@nasa.gov), who has the overall responsibility for this product, with copies to Can Li (Can.Li@nasa.gov).

The subsets of OMSO2 data over many ground stations and along Aura validation aircraft flights paths are also available through the Aura Validation Data Center (AVDC) web site.

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