

## Overview

This document describes the OMI SO<sub>2</sub> 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<sub>2</sub> mass detectable by OMI is about two orders of magnitude smaller than the detection threshold of the legacy Total Ozone Mapping Spectrometer (TOMS) SO<sub>2</sub> data (1978-2005) [[Krueger, et al. 1995](#)]. OMI also enables the detection of anthropogenic SO<sub>2</sub> 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<sub>3</sub> from SO<sub>2</sub>.

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 (~32 days).

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<sub>2</sub> data, the row anomaly manifests itself as positive or negative stripes (discontinuity in SO<sub>2</sub> with cross-track viewing angle). Efforts have been made to flag the affected scenes. SO<sub>2</sub> 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 column density of SO<sub>2</sub> in Dobson Units (1DU=2.69 ·10<sup>16</sup> molecules/cm<sup>2</sup>) obtained by making different assumptions about the vertical distribution of the SO<sub>2</sub>. However, it is important to note that in most cases the precise vertical distribution of SO<sub>2</sub> is unimportant. The users can use either the SO<sub>2</sub> plume height, or the center of mass altitude (CMA) derived from SO<sub>2</sub> vertical distribution, to interpolate between the 4 values:

- Planetary Boundary Layer (PBL) SO<sub>2</sub> column (**ColumnAmountSO2\_PBL**), corresponding to CMA of 0.9 km. **Please check the following section for important updates to the PBL SO<sub>2</sub> data.**
- Lower tropospheric SO<sub>2</sub> column (**ColumnAmountSO2\_TRL**), corresponding to CMA of 2.5 km.
- Middle tropospheric SO<sub>2</sub> column, (**ColumnAmountSO2\_TRM**), usually produced by volcanic degassing, corresponding to CMA of 7.5 km,

- Upper tropospheric and Stratospheric SO<sub>2</sub> column (**ColumnAmountSO2\_STL**), usually produced by explosive volcanic eruption, corresponding to CMA of 17 km.

The accuracy and precision of the derived SO<sub>2</sub> columns vary significantly with the SO<sub>2</sub> CMA and column amount, observational geometry, and slant column ozone. OMI becomes more sensitive to SO<sub>2</sub> above clouds and snow/ice, and less sensitive to SO<sub>2</sub> below clouds. Preliminary error estimates are discussed below (see Data Quality Assessment).

## Important Updates to OMI PBL SO<sub>2</sub> Data

The SO<sub>2</sub> data in **ColumnAmountSO2\_PBL** are now produced with a completely different retrieval algorithm based on principal component analysis (PCA) of the OMI radiance data [Li et al. 2013]. Previously the OMI PBL SO<sub>2</sub> data were produced using the Band Residual Difference (BRD) algorithm [Krotkov et al 2006]. While the BRD algorithm is sensitive to SO<sub>2</sub> 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<sub>2</sub> retrievals and has been implemented for operational production of the next generation OMI standard SO<sub>2</sub> product. **PBL SO<sub>2</sub> data users who have acquired OMSO2 data prior to October 2014 are strongly encouraged to download and use the new OMSO2 data. All SO<sub>2</sub> data fields ending with “BRD” are obsolete and only used for internal diagnostic purposes.**

## Algorithm Description

We use two different algorithms to produce SO<sub>2</sub> column amount data from OMI. The PBL columns are produced using the principal component analysis (PCA) algorithm [Li et al 2013] that are sensitive to pollution near the surface, while TRL, TRM and STL columns are produced with the Linear Fit (LF) algorithm for volcanic SO<sub>2</sub> [Yang et al 2007].

In the PCA algorithm, we apply a principal component analysis technique to radiance data over a presumably SO<sub>2</sub>-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 variance, the second PC explains the second most of 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<sub>2</sub> 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<sub>2</sub> Jacobians, which represents the

sensitivity of the radiances to the SO<sub>2</sub> column ( $\partial N/\partial \Omega_{SO_2}$ ), to the measured Sun-normalized radiances, we can simultaneously obtain estimates of SO<sub>2</sub> column density ( $\Omega_{SO_2}$ ) and coefficients of the PCs ( $\omega$ ):

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

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  $\lambda$ , 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<sub>3</sub> column amount ( $\Omega_{O_3}$ ) from the OMTO3 product [*Bhartia and Wellemeyer*, 2002]. The spectral window includes the strong SO<sub>2</sub> 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<sub>3</sub> absorption due to large slant column O<sub>3</sub> ( $S_{O_3} > 1500$  DU) are filtered out before PCA, given the much smaller expected SO<sub>2</sub> 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<sub>2</sub> 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<sub>2</sub> absorption ( $v_{SO_2}$ ) to be among the first few leading PCs. A correlation analysis between the PCs and the SO<sub>2</sub> 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  $v_{SO_2}$  and collinearity in Eq. 1, and allows reasonable initial estimates of SO<sub>2</sub> ( $\Omega_{SO_2\_ini}$ ) 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  $\Omega_{SO_2\_ini}$  (within  $\pm 1.5$  standard deviations for each orbit/row) to extract a new set of PCs to update Eq. 1, followed by updated retrievals of SO<sub>2</sub>. This step is repeated twice, as the changes in the retrieved SO<sub>2</sub> 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  $S_{O_3} < 100$  DU + min( $S_{O_3}$ ), and two regions north and south of it. These regionally derived PCs more closely match the measurements and help reduce retrieval biases.

The SO<sub>2</sub> Jacobians used in the current version of the 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 ( $30^\circ$ ) and viewing zenith angle ( $0^\circ$ ). For  $\text{SO}_2$ , a climatological profile over the summertime eastern U.S. are used. For  $\text{O}_3$  and temperature, the OMTO3 standard mid-latitude profiles with  $\Omega_{\text{O}_3} = 325$  DU are used. This setup allows direct comparison between the new and old OMI PBL  $\text{SO}_2$  data. In the future, we plan to expand the look-up table for  $\text{SO}_2$  Jacobians to more realistically account for different measurement conditions.

The LF algorithm uses a recently modified version (Version 8.5) of TOMS total ozone algorithm (OMTO3) [Bhartia and Wellemeyer 2002] as a linearization step to derive an initial estimate of total ozone assuming zero  $\text{SO}_2$ . (See [OMTO3 README file](#) for more detail). The residuals at the 10 wavelengths are then calculated as the difference between the measured and computed N-values using a vector forward model radiative transfer code that accounts for multiple Rayleigh scattering, ozone absorption, Ring effect, and surface reflectivity, but assumes no aerosols. Cloudy scenes are treated as mixture of two opaque Lambertian surfaces, one at the terrain pressure and the other at Radiative Cloud Pressure (RCP) derived using OMI-measured Rotational Raman scattering at around 350 nm (see [OMCLDRR README file](#) for more detail). In the presence of  $\text{SO}_2$ , the residuals contain spectral structures that correlate with the  $\text{SO}_2$  absorption cross-section. The residuals also have contributions from errors sources that have not yet been identified. To reduce this interference, a median residual for a sliding group of  $\text{SO}_2$ -free and cloud-free scenes (OMTO3 radiative cloud fraction  $< 0.15$ ) covering  $\pm 15^\circ$  latitude along the orbit track is subtracted for each spectral band and cross-track position [Yang et al 2007].

The LF algorithm uses the corrected residuals as input.  $\text{SO}_2$  produced by volcanic degassing and eruptions can produce large errors in OMTO3 derived total ozone and can make the retrieval highly non-linear. The linear Fit (LF) algorithm was developed to handle such cases. The LF algorithm minimizes different subsets of residuals by simultaneously adjusting total  $\text{SO}_2$ , ozone and includes a quadratic polynomial in the spectral fit. The subsets are determined by the process of dropping the shortest wavelength bands one at a time until the 322nm band is reached. The largest  $\text{SO}_2$  retrieval is reported as the final estimate. The assumed gaseous vertical profiles correspond to the standard OMTO3 ozone profiles. The  $\text{SO}_2$  weighting functions are approximated using OMTO3 layer Efficiency factors in Umkehr layers 0, 1 and 3, for ColumnAmountSO2\_TRL, ColumnAmountSO2\_TRM, and ColumnAmountSO2\_STL data, correspondingly. Treatment of aerosols and clouds is the same as in the OMTO3 algorithm.

## Data Quality Assessment

Errors in OMI  $\text{SO}_2$  data can arise from both the input radiance/residual data and the  $\text{SO}_2$  Jacobians/weighting functions used in retrievals. For the LF algorithm, the “sliding median” empirical residual correction essentially acts as a high-pass filter reducing cross-track and low frequency latitudinal biases, but allowing high frequency (i.e. “scene by

scene”) noise in the residuals to propagate into retrieved background SO<sub>2</sub> data. 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. The noise in PCA retrievals can also be described in a similar fashion.

We provide separate Quality Flags (QF) for each of the products that are based on SO<sub>2</sub> consistency criteria between the individual wavelength pairs. The OMSO2 scene quality flag is an automatic assessment of the SO<sub>2</sub> values for the corresponding scene by the OMSO2 retrieval algorithm. It is used primarily as an indicator of the validity of the retrieved SO<sub>2</sub> 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 work best for large volcanic events, but miss many real PBL and low level degassing emissions. Therefore, independent verification of the real SO<sub>2</sub> 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.** No data filtering is needed for TRM, TRL, and STL data fields. Below are data quality assessments for each SO<sub>2</sub> product after applying the “sliding median” empirical residual correction and ignoring QF (**Note: no sliding median is applied to PBL**). 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<sub>2</sub>-free equatorial Pacific, 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<sub>3</sub>, 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<sub>3</sub> < 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<sub>2</sub> retrieval accuracy also depends on the error in the SO<sub>2</sub> Jacobians. This error is systematic and increases with deviation of the observational conditions from those assumed in the Jacobian calculation. SO<sub>2</sub> will likely be overestimated for remote oceanic regions where SO<sub>2</sub> is transported from source regions and likely located at elevated levels above the PBL. Likewise, SO<sub>2</sub> will also be overestimated for scenes with snow/ice and/or clouds. We plan to expand the look-up table for SO<sub>2</sub> 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<sub>2</sub> 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<sub>2</sub> on the number of PCs included in the fitting. We expect to provide a more complete error estimate in follow-up releases.

**ColumnAmountSO2\_TRL:** Due to increased sensitivity to elevated SO<sub>2</sub>, the 1 sigma noise in TRL data is estimated at ~0.7 DU under optimal observational conditions in the tropics. The data can be used for cloudy, clear and mixed scenes as well as for elevated terrain. However, the TRL data contain filled values when terrain pressure or RCP is less than ~500hPa. In such cases the cloud blocks most of the SO<sub>2</sub>. As a result, the SO<sub>2</sub> weighting function approaches zero, no LF retrieval is done and the fill value is stored in the output.

**ColumnAmountSO2\_TRM** are optimized for typical volcanic degassing from volcanoes with vents at ~5km altitude or above and emissions from effusive eruptions. The standard deviation of TRM retrievals in background areas is about 0.3 DU at low and mid-latitudes. The cloud-related fill values in TRM data occurs only when the OMI measured cloud top is higher than ~8-10 km. Biases in the TRM retrievals due to latitude and viewing angle are removed to the 0.1 DU level by the median residual background corrections. Both the bias and standard deviations increase with solar zenith angle. **We recommend that the TRM retrievals be used for volcanic degassing cases at all altitudes** because the PBL retrievals are restricted to optimal viewing conditions and TRL data are overestimated for high altitude emissions (>3km). In general, SO<sub>2</sub> releases at altitudes less than ~7.5 km will be underestimated, but these errors can be corrected off-line using the averaging kernel [Yang et al 2007] if the actual SO<sub>2</sub> vertical distribution is known.

Analysis of daily OMSO<sub>2</sub> data for degassing volcanoes at high altitude (~5 km) has shown that significant trends in SO<sub>2</sub> burdens, linked to variability of source SO<sub>2</sub> emissions, can be detected [Carn et al., 2008a]. Preliminary surveys of global volcanic OMSO<sub>2</sub> data indicate that the current sensitivity of the algorithm permits detection of volcanoes emitting on the order of 10<sup>3</sup> tons SO<sub>2</sub>/day or more in daily data (under optimal viewing conditions). Detection of weaker sources usually requires temporal averaging of the OMSO<sub>2</sub> data.

**ColumnAmountSO2\_STL** data are intended for use with explosive volcanic eruptions where the cloud is placed in the upper troposphere or stratosphere (UTLS). At these altitudes the averaging kernel is weakly dependent on altitude, so that differences in

actual cloud height from ~17 km produce only small errors. The biases with latitude and viewing angle are generally less than 0.2 DU. The noise level in background data is about 0.2 DU. This sensitivity has permitted tracking of volcanic SO<sub>2</sub> clouds in the UTLS for great distances from the source [e.g., Carn et al., 2007b, Carn et al., 2008b]. Both the bias and standard deviation increase near the northern terminator, similar to but reduced from the TRM results. Artifacts due to ozone profile errors are reduced from the TRM data by about 30%. One should see no fill values due to cloud screening in the STL data.

The LF algorithm still has large error when it comes to high SO<sub>2</sub> loading cases. The LF algorithm as implemented in the v1.1.6 OMSO2 is expected to provide good retrieval when SO<sub>2</sub> loading is less than ~50 DU. When SO<sub>2</sub> loadings are higher than ~100 DU the LF algorithm underestimates the true SO<sub>2</sub> amount, the higher the loading the larger the underestimation [Yang et al 2007]. Comparisons between total SO<sub>2</sub> burdens calculated using OMSO2 and EP-TOMS SO<sub>2</sub> data for volcanic clouds in the UTLS have shown agreement to within 20% for SO<sub>2</sub> column amounts of <100 DU.

## 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<sub>2</sub> 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, OMT03 reflectivity (LER) and independent estimates of the SO<sub>2</sub> vertical columns, as well as a number of ancillary parameters that provide information to assess data quality. Four values of SO<sub>2</sub> 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 Nikolay 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.

## References

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