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 1:45pm 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 minimum 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: http://toms.umbc.edu]. 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 containing 60 binned pixels or scenes per viewing line. 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 11 May 2008 signal suppression (anomaly) has been observed in Level 1B Earth radiance data for scene numbers 39-42 (unit based), but only for northern Latitudes (see OMI instrumental effects). The anomaly manifests itself as positive or negative stripes in SO2 data (discontinuity with cross-track viewing angle). It is recommended not to use the SO2 data for affected scene numbers in northern hemisphere.

For each OMI scene we provide 4 different estimates of the column density of SO_2 in Dobson Units ($1DU=2.69 \cdot 10^{16}$ 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.
- Lower tropospheric SO_2 column (**ColumnAmountSO2_TRL**), corresponding to CMA of 2.5 km.
- Middle tropospheric SO_2 column, (**ColumnAmountSO2_TRM**), usually produced by volcanic degassing, corresponding to CMA of 7.5 km,
- Upper tropospheric and Stratospheric SO_2 column (**ColumnAmountSO2_STL**), usually produced by explosive volcanic eruption, corresponding to CMA of 17 km.

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). Details about software versions and known issues are available in the OMSO2ReleaseDetails file.

Algorithm Description

We use two different algorithms to produce SO_2 column data from OMI. The PBL columns are produced using the Band Residual Difference (BRD) algorithm [Krotkov et al 2006], while TRL, TRM and STL columns are produced with the Linear Fit (LF) algorithm [Yang et al 2007]. Both algorithms use 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 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 ($N=-100*log_{10}(I/F)$, I is Earth radiance and F is solar irradiance) 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 Lamberian 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 SO_2, the residuals contain spectral structures that correlate with the SO_2 absorption cross-section. The residuals also have contributions from other errors sources that have not yet been identified. To reduce this interference, a median residual for a sliding group of SO_2-free and cloud-free scenes (OMTO3 radiative cloud fraction < 0.15) covering $\pm 15^o$ latitude along the orbit track is subtracted for each spectral band and cross-track position [Yang et al 2007].

Both the BRD and LF algorithms use the corrected residuals as their inputs to derive SO_2 column amount. The BRD algorithm works best in presence of anthropogenically produced SO_2, since they do not affect the total ozone derived by the OMTO3 algorithm. This algorithm uses differential residuals at the three wavelength pairs with the largest differential SO_2 cross-sections to maximize sensitivity to anthropogenic emissions in the PBL. Each pair residual is converted to SO_2 slant column density (*SCD*) using differential SO_2 cross-sections data at constant temperature (275 K) [Bogumil et al 2003]. The *SCDs* of the three pairs are averaged and the average *SCD* is converted to the total SO_2 vertical column density (VCD) using a constant air-mass factor (*AMF*) of 0.36. This *AMF* was estimated for cloud- and aerosol-free conditions, using a solar zenith angle of 30^o, nadir viewing direction, a surface albedo of 0.05, a surface pressure of 1013.3hPa, a 325 DU mid-latitude ozone profile and a typical measured summer SO_2 vertical profile over the Eastern US. Krotkov et al [2008] provide an estimate of how the *AMFs* vary with observing conditions**.**

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 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 SO_2 retrieval is reported as the final estimate. The assumed gaseous vertical profiles correspond to the standard OMTO3 ozone profiles. The 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

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_2 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.

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. **A user of OMSO2 data is advised to examine the first bit of the quality flag. If this bit is equal to zero, the retrieved SO_2 value is likely to be good**. But if it is equal to 1, this indicates that during the retrieval, the algorithm has determined that the scene does not exhibit characteristics that are consistent with the presence of SO_2. Also the quality flag includes other information, such the geometrical and geophysical conditions, that are relevant to the quality of SO_2 retrieval. For detailed information about the OMSO2 quality flag, please consult the OMSO2 file specification). 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_2 signal is strongly recommended. Below are data quality assessments for each SO_2 product after applying the "sliding median" empirical residual correction and ignoring QF. 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: **Due to reduced OMI sensitivity to SO_2 in PBL this product should be used only under optimal viewing conditions: radiative cloud fraction <0.2, solar zenith angle < 40^o and near-nadir viewing angles (cross track positions 20 to 40).** The noise standard deviation (sigma) is ~1.5 DU in the tropics, but increases with latitude, viewing and solar zenith angles and total ozone. Given this large noise only plumes from strong anthropogenic sources of SO_2 (such as smelters and coal burning power plants) and from strong regional pollution can be detected in scene data [Carn et al 2007a; Krotkov et al 2008]. Averaging over a larger area or for a longer time reduces the noise but slower than the square root of the number of scenes averaged. The sigma reduces to ~0.8 DU when 4 scenes are averaged and approaches ~0.4 DU with increasing number of averaged scenes. The SO_2 detection limit is roughly twice of the 1 sigma noise.

The SO_2 retrieval accuracy depends on the uncertainty in both *SCD* and in average photon path, characterized by the error in assumed air-mass factor (*AMF*). The *AMF* error is systematic and increases with deviation of the observational conditions from those assumed in the operational algorithm. For cloud-free scenes, the *AMF* can be corrected using OMI slant column ozone (*SCO*) data as described in Krotkov et al [2008]. For large *SCO* values >1500 DU (i.e. high ozone and/or high solar zenith and viewing angles, mostly at high latitudes), the *AMF* becomes very small, so valid PBL SO_2 retrievals are not expected. In addition, aerosols and sub pixel clouds affect the *AMF* in different ways depending on their vertical distribution. Though clouds screen PBL SO_2, we have not attempted to correct for this effect. For this reason we do not recommend using this product when the radiative cloud fraction (RCF) exceeds 0.2.

ColumnAmountSO2_TRL: Due to increased sensitivity to elevated SO_2, the 1 sigma noise in TRL data is reduced to ~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_2. As a result, the SO_2 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_2 releases at altitudes less than ~7.5 km will be underestimated, but these errors can be corrected off-line using the averaging kernel [Yaong et al 2007] if the actual SO2 vertical distribution is known.

Analysis of daily OMSO2 data for degassing volcanoes at high altitude (~5 km) has shown that significant trends in SO_2 burdens, linked to variability of source SO_2 emissions, can be detected [Carn et al., 2008a]. Preliminary surveys of global volcanic OMSO2 data indicate that the current sensitivity of the algorithm permits detection of volcanoes emitting on the order of 10^3 tons SO_2/day or more in daily data (under optimal viewing conditions). Detection of weaker sources usually requires temporal averaging of the OMSO2 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_2 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_2 loading cases. The LF algorithm as implemented in the v1.1.1 OMSO2 is expected to provide good retrieval when SO_2 loading is less than ~50 DU. When SO_2 loadings are higher than ~100 DU the LF algorithm underestimates the true SO_2 amount, the higher the loading the larger the underestimation [Yang et al 2007]. Comparisons between total SO_2 burdens calculated using OMSO2 and EP-TOMS SO_2 data for volcanic clouds in the UTLS have shown agreement to within 20% for SO2 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_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 Kai Yang (Kai.Yang.1@gsfc.nasa.gov) Arlin J. Krueger (akrueger@umbc.edu), and Simon Carn (scarn@umbc.edu).

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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