Making Earth Science Data Records for Use in Research Environments (MEaSUREs)

README Document for

OMPS_NPP_NMSO2_PCA_L2
OMPS NPP Nadir Mapper SO2 Level 2 Product Based on PCA Algorithm

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Revision History

09/13/2019, NMSO2-PCA-L2 product updated from version 1.1 to version 1.2, introducing a new volcanic SO$_2$ flagging scheme.
TABLE OF CONTENTS

1. INTRODUCTION
   1.1 OMPS_NPP_NMSO2_PCA_L2 Product
   1.2 OMPS/SNPP Nadir Mapper
   1.3 Science Background

2. PRINCIPAL COMPONENT ANALYSIS SO2 ALGORITHM
   2.1 General Description
   2.2 PBL SO2 Retrieval
   2.3 Volcanic SO2 Retrieval
   2.4 Data Quality Assessment and Data Filtering
   2.5 Updates in Version 1.2

3. DATASET ORGANIZATION
   3.1 File Naming Convention
   3.2 File Format and Structure
   3.3 Key Science Datasets

4. DATA CONTENTS
   4.1 Global Attributes
   4.2 Dimensions
   4.3 Datasets

5. CONTACTS

6. REFERENCES
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 (SO₂) 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 data since January 2012. As part of the NASA’s Making Earth System Data Records for Use in Research Environments (MEaSUREs) program, the Goddard Earth Science (GES) Data and Information Data Center (DISC) has released a new SO₂ 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 standard Aura/OMI (Ozone Monitoring Instrument, launched in 2004) SO₂ product produced with the same PCA algorithm, and provides continuity between OMI and the follow-up OMPS instrument aboard the NASA/NOAA JPSS-1 satellite (scheduled for launch in November 2017).

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 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

SO₂ 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 SO₂ 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 SO₂ began with Nimbus-7 Total Ozone Mapping Spectrometer (TOMS, Kruger, 1983). With measurements only at six discrete wavelengths, the TOMS SO₂ data record is generally limited to large volcanic eruptions. Starting from the 1990s, hyperspectral UV measurements made by instruments such as GOME (Global Ozone Monitoring Experiment) allow SO₂ absorption features to be more clearly separated from interfering processes, enabling the detection of anthropogenic SO₂ signal from space (e.g., Eisinger and Burrows, 1998). Since 2004, Dutch-Finnish Ozone Monitoring Instrument (OMI) onboard NASA’s polar orbiting Aura satellite has been providing global monitoring of both anthropogenic and volcanic SO₂ with increased spatial resolution. The previous NASA standard OMI SO₂ 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\textsubscript{2} product (released in 2014 for anthropogenic SO\textsubscript{2} and in 2016 for volcanic SO\textsubscript{2}) is based on the Principal Component Analysis (PCA) algorithm (Li et al., 2013; 2017) that offers significantly improved data quality. NMSO2-PCA-L2 is based on the same PCA retrieval algorithm that has been implemented for Aura/OMI.

2. PRINCIPAL COMPONENT ANALYSIS SO\textsubscript{2} ALGORITHM

2.1 General Description

This section describes the Principal Component Analysis (PCA) SO\textsubscript{2} algorithm and its implementation with SNPP/OMPS. The algorithm has been described in detail elsewhere (Li et al., 2013; 2017) 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 derive 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\textsubscript{2} spectral fitting to reduce their interferences. It should be noted that BUV instruments such as OMI and OMPS have different sensitivities to SO\textsubscript{2} at different altitudes. In the absence of such information on the SO\textsubscript{2} plume height, for each OMPS pixel, the NMSO2-PCA-L2 provides five estimates of the total SO\textsubscript{2} Vertical Column Density (VCD) in Dobson Units (1 DU = 2.69 \cdot 10^{16} \text{ molecules/cm}^2), with each corresponding to a different assumed SO\textsubscript{2} cloud height or Center of Mass Altitude (CMA). All five VCD values represent the estimated total SO\textsubscript{2} burden within the entire atmospheric column. Therefore they should not be interpreted as partial column amounts within different layers or parts of the atmosphere. The five estimates are provided
so that data users may select the one or interpolate between the two estimates that are most representative of the conditions for a particular case of interest.

2.2 PBL SO$_2$ Retrieval

The Planetary Boundary Layer (PBL) SO$_2$ in NMSO2-PCA-L2 is an estimated SO$_2$ VCD assuming that SO$_2$ is predominantly in the PBL or the lowest one km of the atmosphere. It is recommended for use in studies on near-surface pollution. 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 $v_i$) for the spectral range 310.5-340 nm from the sun-normalized BUV radiance spectra. 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 the 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 ($\Omega_{SO2}$) and the coefficients of the PCs ($\omega$) by fitting the first $n_v$ (up to 15 non-SO$_2$) PCs and the SO$_2$ Jacobians ($\partial N / \partial \Omega_{SO2}$) to the measured radiance spectrum (in this case the quantity $N$, which is the scaled logarithm of the sun-normalized radiances, $I$):

$$N(\omega, \Omega_{SO2}) = \sum_{i=1}^{n_v} \omega_i v_i + \Omega_{SO2} \frac{\partial N}{\partial \Omega_{SO2}} \quad (1)$$

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 $\Omega_{SO2}$, and were pre-calculated with a radiative transfer code. For the current NMSO2-PCA-L2 PBL SO$_2$ VCD data, we use a fixed SO$_2$ Jacobian spectrum in Eq. (1), 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 O₃ and temperature profiles (with O₃ VCD = 325 DU). This simplification may lead to biases under certain conditions and data filtering is recommended before analysis (see below).

2.3 Volcanic SO₂ Retrieval

To facilitate studies on volcanic SO₂, NMSO2-PCA-L2 provides SO₂ VCD estimates assuming SO₂ 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 violent volcanic eruptions. For volcanic SO₂ retrievals, we use PBL SO₂ (section 2.2) and the Simple Lambertian Equivalent Reflectivity (SLER or R) derived from TOA radiances for each pixel as input. The SO₂ Jacobians as a function of solar zenith angle (θ₀), viewing zenith angle (θ), and relative azimuth angle (ϕ) can be calculated with the following equation:

\[
\frac{\partial I}{\partial \Omega_{\text{SO}_2}} = \frac{\partial I_0(\theta_0, \theta)}{\partial \Omega_{\text{SO}_2}} + \frac{\partial I_1(\theta_0, \theta)}{\partial \Omega_{\text{SO}_2}} \cos \phi + \frac{\partial I_2(\theta_0, \theta)}{\partial \Omega_{\text{SO}_2}} \cos 2\phi + \frac{R}{(1-R S_b)} \frac{\partial L_r(\theta_0, \theta)}{\partial \Omega_{\text{SO}_2}} + \frac{R^2 L_r(\theta_0, \theta)}{(1-R S_b)^2} \frac{\partial S_b}{\partial \Omega_{\text{SO}_2}}
\]  

(2)

Here \( I_0, I_1, \) and \( I_2 \) represent the atmospheric contribution to the radiances (I). \( R L_r \) represents the TOA radiance that is reflected once from the surface and transmitted through the atmosphere, and \( (1 - R S_b) \) 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. In addition, SO₂ Jacobians also depend on the amount and vertical profile of SO₂ and O₃.

In the retrieval algorithm, the SO₂ Jacobians are interpolated from a set of pre-calculated lookup tables for 21 climatology O₃ profiles and four presumed SO₂
profiles (i.e., TRL, TRM, TRU, and STL). The nodes of $\theta_0$ (SZA), $\theta$ (VZA) and SO$_2$ in the lookup table are given in Table 1.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Nodes</th>
</tr>
</thead>
<tbody>
<tr>
<td>SZA</td>
<td>0°    15° 30° 45° 60° 70° 77° 81°</td>
</tr>
<tr>
<td>VZA</td>
<td>0°    15° 30° 45° 60° 70° 75° 80°</td>
</tr>
<tr>
<td>SO$_2$ (DU)</td>
<td>0  1  5  10 50 100 200 300 400 500 600 700 800 900 1000</td>
</tr>
</tbody>
</table>

For each OMPS pixel, the SO$_2$ Jacobians are first calculated from exact observational geometry, scene reflectivity, $R$, and PBL SO$_2$ for an initial estimate of the volcanic SO$_2$ VCDs. 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 (15). 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 estimates.

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 comparison between NMSO2-PCA-L2 and the OMI PCA SO$_2$ data, and found generally good agreement between the two products (Li et al., 2017; Zhang et al., 2017), despite large differences in instrument spectral and spatial resolution.

For data analysis, we recommend that all pixels with large solar zenith angle (SZA > 70) or near the edge of the swath (rows 1-2 and 35-36) or significantly 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.

**ColumnAmountSO2_PBL:** As a measurement of retrieval noise, the pixel-level standard deviation is ~0.2-0.3 DU over the presumably SO$_2$-free equatorial Pacific for PBL SO$_2$. For PBL SO$_2$, because of the simplification in Jacobians mentioned above, we also recommend that only snow/ice free pixels with relatively small RadiativeCloudFraction (< 0.3) be used.

**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 for high latitudes. The data can be used for cloudy, clear and mixed scenes as well as for elevated terrain, but will overestimate SO$_2$ amounts if SO$_2$ cloud altitude is higher than 3 km. The TRL data can be used for studies of volcanic degassing.

**ColumnAmountSO2_TRM:** The standard deviation of TRM retrievals in 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$_2$ amounts if SO$_2$ cloud altitude is higher than ~8 km.
**ColumnAmountSO2_TRU** data are intended for use for explosive volcanic eruptions where SO$_2$ is injected into the upper troposphere. The standard deviation over background areas is $< 0.1$ DU for all latitudes for TRU data. The TRU data can be used for investigating SO$_2$ clouds from explosive eruptions in upper troposphere and tropopause in mid- and high latitudes, but will overestimate SO$_2$ amounts if SO$_2$ cloud CMA is higher than $\sim 13$ km.

**ColumnAmountSO2_STL** data are intended for use for explosive volcanic eruptions where SO$_2$ is injected directly into the lower stratosphere at 16-20km. STL data will underestimate total SO$_2$ amounts for lower SO$_2$ cloud altitudes. The standard deviation over background areas is $< 0.1$ DU for all latitudes for STL data.

### 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 version 1.1 NMSO2-PCA-L2 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 version 1.2, 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 version 1.2 NMSO2-PCA-L2 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 version 1.2 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) version 1.1 and (b) version 1.2 of the NMSO2-PCA-L2 product.

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_v1.0_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 (1.0)
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 five key science datasets in the science data group in each NMSO2-PCA-L2 product file that correspond to the five estimates of the total vertical column amount (VCD) of \( \text{SO}_2 \) assuming specific cloud height.

3.3.1 \textit{ColumnAmountSO2\_PBL}

\textit{ColumnAmountSO2\_PBL} is the estimated total VCD of \( \text{SO}_2 \) in DU assuming that the observed \( \text{SO}_2 \) lies within the lowest kilometer of the atmosphere.

3.3.2 \textit{ColumnAmountSO2\_TRL}

\textit{ColumnAmountSO2\_TRL} is the estimated total VCD of \( \text{SO}_2 \) in DU assuming a center of mass altitude of 3 km.

3.3.3 \textit{ColumnAmountSO2\_TRM}

\textit{ColumnAmountSO2\_TRM} is the estimated total VCD of \( \text{SO}_2 \) in DU assuming a center of mass altitude of 8 km.

3.3.4 \textit{ColumnAmountSO2\_TRU}

\textit{ColumnAmountSO2\_TRU} is the estimated total VCD of \( \text{SO}_2 \) in DU assuming a center of mass altitude of 13 km.

3.3.5 \textit{ColumnAmountSO2\_STL}
ColumnAmountSO2_STL is the estimated total VCD of SO2 in DU assuming a center of mass altitude of 18 km.

4. DATA CONTENTS

Each NMSO2-PCA-L2 product file contains global attributes, dimensions, an ancillary data group, a geolocation data group, and a science data group.

4.1 Global Attributes

There are 42 global attributes in each NMSO2-PCA-L2 product file as shown in Figure 2.

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<td>String, length = 18</td>
<td>Scalar</td>
</tr>
</tbody>
</table>
4.2 Dimensions

There are four dimensions in each NMSO2-PCA-L2 product file:

nTimes - The dimension representing the along-track-line number.
nWavel2 - The dimension representing the wavelengths for the fitting windows.
nWavel3 - The dimension representing the wavelengths for SLER and dN/dR.
nXtrack - The dimension representing the cross-track-position number.

4.3 Data Fields

4.3.1 Ancillary Data
There are two datasets, CloudPressure and TerrainPressure, in the ancillary data group in each NMSO2-PCA-L2 product file as shown in Figure 4.

![Ancillary Data Group](image)

Figure 4. Ancillary Data Group

4.3.2 Geolocation Data

There are eleven datasets in the geolocation data group in each NMSO2-PCA-L2 product file as shown in Figure 5.
4.3.3 Science Data

There are 20 datasets in the science data group in each NMSO2-PCA-L2 product file as shown in Figure 6.
5. CONTACTS

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6. REFERENCES


