

OMNO2 README File

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Data Product Version 1.0.5

Overview

Nitrogen dioxide is an important chemical species in both the stratosphere, where it plays a key role in ozone chemistry, and in the troposphere, where it is a precursor to ozone production. In the troposphere, it is produced in various combustion processes and in lightning. It is a significant indicator of poor air quality, and its measurement is a key objective of the OMI project.

This document provides a brief description of the OMI Nitrogen Dioxide (NO₂) data product, OMNO2. The present version of this document refers to the Collection 3 Release (Version 1.0.5) of this data product, November 2007. OMNO2 contains the observed slant column NO₂ (total amount along the optical path from the sun into the atmosphere, and then toward the satellite), the total vertical column NO₂ [cm⁻²], and the estimated tropospheric portion of the total column NO₂ [cm⁻²]. Other ancillary data are also provided in the OMNO2 file, including data quality flags, measures of precision, and quality assurance (QA) information.

An estimate of the NO₂ column hidden by any clouds in the OMI field of view has been included in the OMNO2 data product. At the user's discretion, this "ghost column" can be added to the observed column amounts (defined below in the section "Description of Retrieved NO₂ Columns") to estimate total column amounts above ground. The ghost column is not a tabulated a priori, or climatological, amount, but is computed from the measured NO₂ column above the clouds and the assumed a priori NO₂ profile *shape*. Uncertainties in the ghost column are typically large – on the order of 100%.

Application

This document applies to the current public release of the OMNO2 product, version 1.0.5, November 2007. This product is archived as Collection 3. The software versions used to produce the data are presented in the table below.

OMCLDO2	V1.0.2
OMNO2A	V1.0.5
OMNO2B	V1.0.0
OMNO2	V0.9.33

Algorithm Description

The basic algorithm for the retrieval of total column and tropospheric NO₂ from OMI data is described by *Boersma et al.* [2001] in *Volume IV of the OMI Algorithm Theoretical Basis Document (ATBD)*, available at

http://eospsso.gsfc.nasa.gov/eos_homepage/for_scientists/atbd/docs/OMI/ATBD-OMI-04.pdf

Further information about the algorithm and its development may also be found in *Bucsela et al.*, [2006]. However, some of the data fields in the OMNO2 product differ from those described in these references (see “Description of Retrieved NO₂ Columns” below).

The user is strongly advised to read the section “**Known Issues**” below.

The algorithm is divided into three processes, each performed by a separate program, or Product-Generating Executive (*PGE*). The end result is the creation of the OMNO2 data product from the OMI Level 1B product. Here we briefly describe each PGE.

The first PGE (PGE-A) performs a least-squares fit based on the ratio of the measured earthshine radiance spectrum to a solar irradiance spectrum. A static reference solar spectrum is used to compute this ratio. The static solar spectrum is an average over all the daily Sun observations from OMI in the year 2005. This approach has resulted in much smaller dark current-related stripes, compared to those seen in earlier versions of the data.

The functions fitted to the spectral ratio are laboratory-measured trace gas spectra, a reference Ring spectrum [*Chance and Spurr*, 1997] and the coefficients of a polynomial function to model the spectrally slowly varying components of scattering by clouds and aerosols and reflection by the Earth’s surface. The fitting algorithm uses the Differential Optical Absorption Spectroscopy (DOAS) method, and is applied in the spectral range 405nm to 465nm. In the current version, the only trace gas absorption spectra considered are those of NO₂ [*Vandaele et al.*, 1998], O₃ [*Burrows, et al.*, 1999] and H₂O [*Harder and Brault*, 1997]. The trace gas absorption spectra actually used were produced by convolving high-resolution, laboratory-measured absorption spectra with the measured OMI slit function. The result of the spectral fit is a slant column density (SCD) for each OMI pixel.

The second PGE (PGE-B) computes the air-mass factors (AMFs), defined as the ratio of the SCD to the vertical column density (VCD) of NO₂. AMFs depend upon a number of parameters including viewing geometry, surface albedo and the shape (not magnitude) of the NO₂ vertical profile. AMFs are calculated using both **unpolluted** (stratospheric and a small amount of upper tropospheric) and **polluted** (lower tropospheric) NO₂ profiles. For each location, the algorithm uses a single mean unpolluted profile derived from the GSFC-CTM and a geographically gridded set of annual mean polluted profiles obtained from the GEOS-CHEM model (see Fig. 1). The method of calculation is similar to that described by

Palmer, et al. [2001], and uses pre-calculated altitude-dependent AMFs, which are stored in look up tables. For each profile, AMFs are derived for clear and cloudy conditions. Clouds are represented as opaque Lambertian reflectors with an albedo of 0.8. A radiance-weighted sum of the two is used for partly cloudy conditions. The cloud information (cloud fraction and cloud pressure) is obtained from the OMCLDO2 cloud product. The AMFs will be applied in the third PGE to convert the SCDs into VCDs.

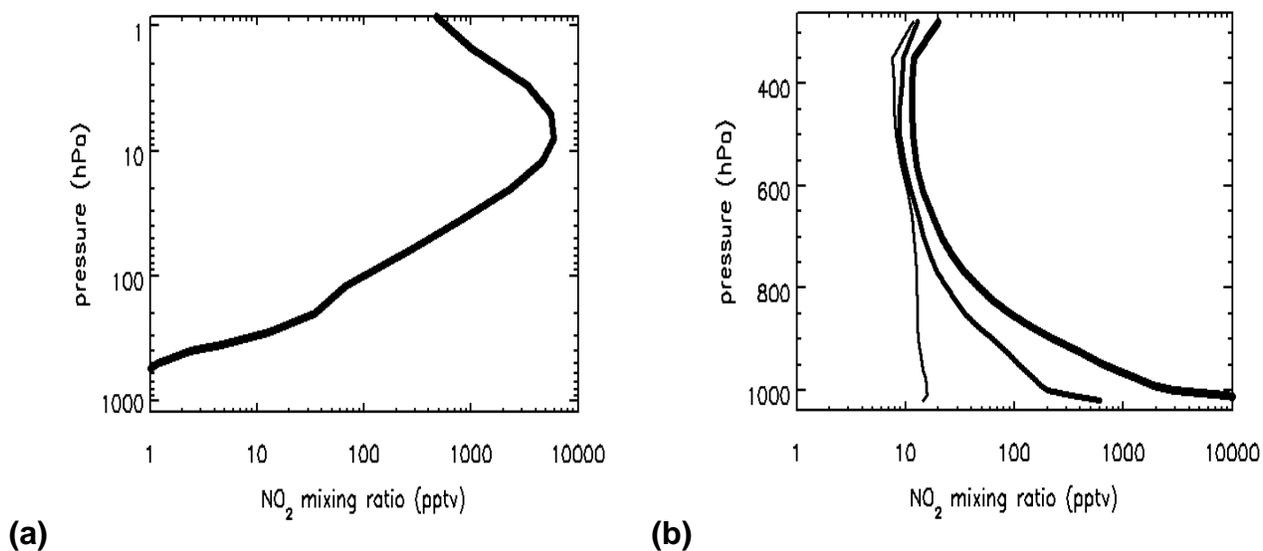


Figure 1: NO₂ concentration profiles used in the calculation of the air mass factors (AMFs). Shown are the unpolluted profile (a) and three examples of polluted profiles (b) for low, moderate and high levels of pollution.

The third PGE (PGE-C) derives an initial estimate of the NO₂ VCD, V_{init} , by dividing the SCD by an unpolluted AMF, and assembles all the data collected within ± 12 hours of the target orbital data granule. Areas shown by GEOS-CHEM to contain climatologically high tropospheric NO₂ amounts are then masked, and the remaining regions are smoothed in latitude bands. The smoothing algorithm employs a “boxcar” smoothing over a 9° latitude band, followed by a zonal planetary wave smoothing up to wave-2. At a given geographic location, the OMI pixels selected for the smoothing are those with the smallest AMFs and slant-column uncertainties. The result is the column amount V_u , which represents the smoothly varying background level of NO₂, including the tropospheric background contribution, and is used in the algorithm as an upper limit on the unpolluted NO₂ column. Pixels for which V_{init} exceeds V_u are assumed to be polluted. The polluted VCD, V_p , is calculated as the difference $V_{init} - V_u$ times the ratio of the unpolluted AMF to the polluted AMF for the pixel. The total column for that pixel is then the sum of V_p and V_u . For all other pixels, the total column is taken to be V_{init} .

Description of Retrieved NO₂ Columns

The Level-2 data file in the Public Release contains four main types of NO₂ vertical column amounts.

- (1) *ColumnAmountNO2* (V^{obs})= the total observed vertical column density above ground.
- (2) *ColumnAmountNO2Trop* (V_{trop}^{obs})= tropospheric observed vertical column density (integrated from ground to 150 mb).
- (3) *ColumnAmountNO2Polluted* (V_p^{obs})= polluted observed vertical column density (integrated from ground to 250 mb).
- (4) *ColumnAmountNO2BelowCloud* (V_{ghost}) = vertical column density hidden by clouds.

In these definitions, the term *observed* refers to the amount of NO₂ that can be seen from above the atmosphere. The observed amount depends on the vertical distribution of NO₂, the pressure level of the cloud top and the effective cloud fraction. For example, if the effective cloud fraction (based on the assumed 80% cloud albedo) is 50%, then the observed column is half the column density above ground plus half the column density above the cloud top. The Level-2 data also contains an estimate of the column amount below any clouds in the field of view. This amount is sometimes called the “ghost column”, and is named *ColumnAmountNO2BelowCloud* in the OMNO2 data product.

Adding the ghost column, V_{ghost} , to V^{obs} , V_{trop}^{obs} , or V_p^{obs} gives the corresponding complete column between the ground and the satellite, e.g.

$$V_{trop} = V_{trop}^{obs} + V_{ghost}$$

For studies comparing OMI with other measured or modeled tropospheric NO₂ columns, it is generally advisable to add the ghost column to the OMI data, particularly when skies are mostly clear to partly cloudy. For studies involving NO₂ in the mid-to-upper troposphere – e.g. NO₂ from lightning sources, or NO₂ observed under overcast conditions - the ghost column is generally a poor estimate of the below-cloud amount and should be omitted. In either case, the use or non-use of the ghost column should be consistent throughout the study.

The quantity *ColumnAmountNO2Polluted* is given only in cases where NO₂ exceeds background levels ($V_{init} - V_u > 0$). In all other cases, fill values are stored. The fill value is the OMI standard fill value, equal to -2^{100} . *ColumnAmountNO2Polluted* is the magnitude of the column above the background, computed assuming that the origin of the excess NO₂ is pollution. Models show pollution affects altitudes mainly below about 250 mb. *ColumnAmountNO2Trop* is defined as the NO₂ vertical column between ground and the estimated mean tropopause pressure of 150 mb. Where the polluted column is defined, *ColumnAmountNO2Trop* is obtained by adding 5% (*TropFractionUnpolluted*) of V_u to *ColumnAmountNO2Polluted*. Elsewhere, *ColumnAmountNO2Trop* is just 5% of the total column.

Although not given explicitly, the *unpolluted* and *stratospheric* columns can be found by subtracting, respectively, the polluted and tropospheric columns from the total column. Note that for cases of measurable pollution ($V_{init} - V_u > 0$), the unpolluted column amount is also equal to V_u . For all other cases, the unpolluted column is defined to be the total column (which is also the initial column in such cases). The VCDQualityFlags data item contains a one-bit flag that indicates whether each pixel was treated as polluted or unpolluted.

Note that the NO₂ fields described here are somewhat different from those discussed in Bucsele et al. [2006]. In that paper, the unpolluted column amount is referred to as “stratospheric” NO₂, and the polluted column amount is called “tropospheric” NO₂. In the OMNO2 data product, tropospheric NO₂ means the polluted amount plus the 5% of the unpolluted column. Another difference is that *Bucsele et al.* describe retrieval of the complete above-ground column amounts. In OMNO2, only the *observed* columns are explicitly given. The complete columns are obtained by adding the ghost column to the total, tropospheric and polluted columns, as described above.

Data Quality Assessment

The quality of the data in this release is currently being established by independent measurements in ongoing validation campaigns from ground-, aircraft-, and satellite-based instruments. An overview of the validation results to date are presented in *Celarier, et al., (2008)*. The principal findings from those validation efforts are summarized in the following table.

Summary of validation study results for OMI NO2 data product					
Instrument	Column	Group	OMI, rel. to GB	Uncert.	Remarks
SAOZ	Strat.	CNRS	-14%	±10%	As large as 25% in tropics
MAX-DOAS	Trop.	BIRA, etc.	-15%	—	Large scatter in the data.
MF-DOAS	Trop.	WSU	-19%	±11%	Very small <i>N</i> .
Aircraft <i>in situ</i>	Trop.	UC, GSFC	-15%	±10%	Large scatter.
Brewer	Total	GSFC	-33%	—	Large <i>N</i> , large scatter.
Pandora-1	Total	GSFC	-15%	—	Very small <i>N</i> , small data range.
DS-DOAS	Total	BIRA	-16%	±5%	Small <i>N</i> , large scatter.
FTUVS	Total	JPL	-23%	±41%	Small <i>N</i> , significant apparent bias, but good correlation.

Some data quality issues are described in the Data Quality document found at http://toms.gsfc.nasa.gov/omi/no2/OMNO2_data_quality.pdf.

An overview of some of the validation efforts may be found in the presentation http://earth.esa.int/workshops/atmos2006/participants/330/pres_330_kroon.pdf.

Stratospheric amounts are in reasonable agreement with climatological measurements from the Halogen Occultation Experiment (HALOE) instrument aboard the Upper Atmosphere Research Satellite (UARS) and with model calculations from the NASA/GSFC chemical transport model (CTM). Tropospheric amounts are generally consistent with the GEOS-CHEM model and indicate prominent sources near urban areas.

The data product includes estimates of uncertainties associated with the various geophysical quantities. The uncertainty estimates have been improved since the provisional release of the OMI data. However, these estimates may not account for all actual sources of random or systematic errors. We anticipate further improvements through the validation process and in understanding the probability distributions of the underlying data and the algorithmic sensitivity to the data.

Known Issues

As a result of unforeseen characteristics of the OMI CCD detector, most retrieved data products show a varying cross-track anomaly: The average value along any orbital track at one cross-track position may differ significantly from that along nearby cross-track positions, resulting in the appearance of "stripes" when the data are displayed on a map. This artifact mostly arises from the performance of the CCD detectors themselves, and, in particular, the dark current. The current version uses a static solar irradiance spectrum. This, in addition to the use of daily updated operational parameter files (OPF) in the Level 0 to Level 1B processing has resulted in Level 2 files that show considerably less striping. A *post-hoc* de-striping step is used to remove any residual striping. This step may be removed in a future version of the algorithm. The decision about whether to continue de-striping or not is awaiting a careful analysis of the data.

The third PGE performs a "de-striping" of NO₂ column amounts by adjusting the mean SCD for a given cross-track position to the mean value at all positions. The current version of the de-striping algorithm computes the mean SCD and the mean initial AMF for each cross-track position from 24-hours of data using measurements obtained at latitudes between $\pm 55^\circ$. These are used to generate a set of 60 correction constants, one for each cross-track position, which are subtracted from the SCD values before computation of the vertical columns. The user should note that the slant columns (*SlantColumnAmountNO2*) actually stored in the Level-2 file are from the original spectral fit and have *not* been de-striped. However the all stored vertical columns, with the exception of *ColumnAmountNO2Initial*, have been de-striped.

Though the de-striping procedure almost certainly introduces an unknowable systematic bias in the retrieved NO₂ VCDs, which could vary from orbit to orbit, if the residual striping of the data before this step is taken is small, such a bias should be very small.

The air mass factors are computed in PGE-B using a look-up table from radiative transfer calculations. The calculations are performed on a 6-dimensional grid of pressures, solar zenith angles, viewing zenith angles, relative azimuth angles, albedos and surface pressures, and the algorithm interpolates between grid points. A finer grid is planned for implementation in the next version of the algorithm. Use of the current coarse grid can cause errors in the polluted AMF, and hence the retrieved polluted and tropospheric column amounts, as large as 10% relative to the fine grid.

The user is referred to the **Release Notes** for additional information and cautions pertaining to the use and interpretation of the data:

http://toms.gsfc.nasa.gov/omi/no2/OMNO2_release_notes.pdf.

Product Description

A single OMNO2 product file contains all OMI measurements on the sunlit portion of the Earth, for one Aura orbit. During one orbit OMI performs approximately 1650 measurements, which take 2 seconds each. In the global observation mode, 60 across track ground pixels are measured simultaneously during a measurement. These 60 measurements cover the ~2600 km-wide OMI ground swath. Fig. 2 shows that due to optical aberrations and the asymmetric alignment between the instrument's optical axis and the spacecraft axes, the ground pixels are not symmetrically aligned with respect to the orbital plane.

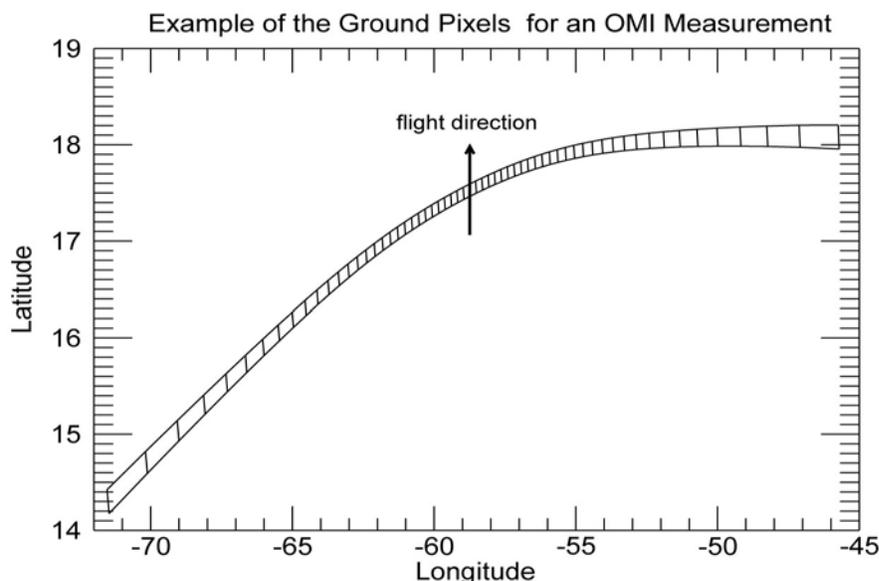


Figure 2: The position of 60 ground pixels for an OMI measurement in the tropics. Note that the x and y axes cover different distances on the Earth's surface. The arrow shows the satellite trajectory

The latitude and longitude provided with each ground pixel represent the location of the center of each pixel on the ground. Fig. 3 gives the size of the ground pixels, as a function of pixel number in the across track direction. Although the pixels also increase in the flight direction when going off nadir, this effect is much smaller and may be neglected for most applications.

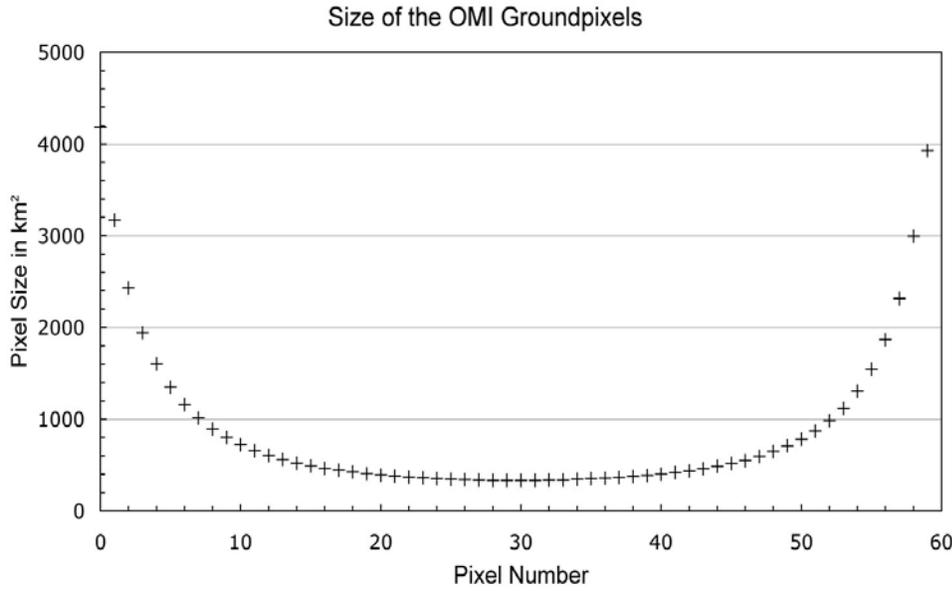


Figure 3: The size of the OMI ground pixels, as a function of the across track pixel number

The OMNO2 product is written as an HDF-EOS5 swath file. For a list of tools that read HDF-EOS5 data files, please visit this link:

<http://disc.gsfc.nasa.gov/Aura/tools.shtml>,

A single OMNO2 file contains information retrieved from each OMI pixel over the sun-lit portion of one Aura orbit. The data are ordered in time. The information provided in these files includes latitude, longitude, a set of viewing angles (solar zenith and solar azimuth; viewing zenith and viewing azimuth), column amounts of NO₂, intermediate quantities used in the calculation, such as AMFs and coefficients of the smooth NO₂ field, and a large number of ancillary parameters that provide information to assess data quality. Among the latter are several data quality flag fields (ground pixel quality, measurement quality, fit quality, AMF quality, and unpolluted field quality). These should be examined to assess the quality of individual measurements, particularly for inter-comparison studies. A two-bit summary flag is also provided to indicate the overall quality of the data for a given pixel. These two bits are the least-significant bits of the vcdQualityFlag data item in a Level 2 file. The following table gives the values of the summary flag.

Flag Value	Meaning
0	Best quality data.

1	(not used)
2	Poor quality data (uses values that came with warnings)
3	Data should not be used.

The simplest way to use the summary flag is to use the least significant bit only: If vcdQualityFlag is read as an integer, then the data should be used only if that integer is even.

For a complete list of fields and ancillary data contained in the OMNO2 file, please read the OMNO2 data product specification http://toms.gsfc.nasa.gov/omi/no2/OMNO2_data_product_specification.pdf.

Users who are not interested in the detailed information provided in OMNO2 dataset, may wish to use one of the several gridded products that are routinely produced using the OMNO2 dataset. A Level 3 (gridded, using weighted-averages of columns within each grid cell) product is available in text or HDF format. A level 3G data set is also available. This is a gridded data set where each grid cell contains a "stack" of Level 2 data for every OMI field-of-view that fell within that cell. Only a subset of the full Level 2 data are included, but enough data is present in the Level 3G data, that the user could easily find the corresponding data in the OMNO2 files. Full OMNO2 data, as well as subsets of these data over many ground stations and along Aura validation aircraft flights paths are available to those investigators who are associated with the various Aura science teams through the Aura Validation Data Center (AVDC) website, <http://avdc.gsfc.nasa.gov/>. Bojan Bojkov Bojan.Bojkov@avdc.gsfc.nasa.gov is the point of contact at the AVDC.

Reporting Problems and Requesting Information

The following is a summary of links to current documentation for OMNO2:

http://toms.gsfc.nasa.gov/omi/no2/OMNO2_readme.pdf
http://toms.gsfc.nasa.gov/omi/no2/OMNO2_release_notes.pdf
http://toms.gsfc.nasa.gov/omi/no2/OMNO2_data_quality.pdf
http://toms.gsfc.nasa.gov/omi/no2/OMNO2_data_product_specification.pdf

To report problems, or pose questions and comments related to the OMNO2 algorithm, data quality, and file structure, please send electronic mail to omno2@ltpmail.gsfc.nasa.gov. Additional questions may be directed to the principal points of contact for OMNO2: James F. Gleason gleason@redwind.gsfc.nasa.gov, and J. Pepijn Veefkind veefkind@knmi.nl.

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