OMNO2 README Document
Data Product Version 3.0

The OMI Nitrogen Dioxide Algorithm Team *

September 2016
Document Version 7.0

Abstract

This README file describes the version 3.0 release of the OMI NO_2 Standard Product, OMNO2, the version 3.0 release of the OMI NO_2 gridded Level-2 (OMNO2G), and the version 3.0 release of the gridded OMNO2d product produced from it.

Species	Nitrogen Dioxide (NO_2)
Data Version	Standard Product, v3.0
Version Release Date	August 2016
Retrieved Quantities	Total slant column density Total vertical column density Stratospheric column density Tropospheric column density
Spatial Resolution	13 km x 24 km (at nadir)
Global Coverage	Approximately daily
Date Range	2004/10/01–Present
Data Screening	See data quality flags in L2 data files
Data Location	http://disc.sci.gsfc.nasa.gov/Aura/data-holdings/OMI
Point of Contact	Nickolay A. Krotkov NASA/Goddard Space Flight Center nickolay.a.krotkov@nasa.gov 301-614-5553

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Contents

List of Tables

1 Executive Summary

The OMI NO_2 algorithm retrieves estimated columns (total, stratospheric, and tropospheric) of nitrogen dioxide from OMI Level-1B calibrated radiance and irradiance data. The current version, 3.0, improves on the retrievals in the previous published version, 2.1 (July 2012) in a number of significant ways. The previous algorithms (1, 2.0, 2.1) were designed to infer as much information as possible about atmospheric NO_2 from the OMI measurements, with the minimum possible dependence on model simulations. This approach has continued with the development of the version 3.0 product.

OMNO2 versions 2.0 and 2.1 represented a significant advance over version 1 [Bucsela et al., 2006, Celarier et al., 2008], and were in greatly improved agreement with independent NO_2 measurements [Bucsela et al., 2013, Lamsal et al., 2014]. During the three years since the version 2.1 release, research at NASA and other institutions has led to significant conceptual and technical improvements in the retrieval of NO_2 from space-based measurements, which have guided the development of the current version.

1.1 Improvements

The principal improvements in version 3.0 include:

1. An improved DOAS algorithm for retrieving slant column densities (SCD). The key features of the algorithm are:
   (a) Iterative subtraction of Ring effect signal–which is usually much larger than the trace gas signals–prior to sequential trace gas retrieval;
   (b) Independent, very accurate registration of wavelength scales between radiance and irradiance spectra;
   (c) Removal of residual spectral structure;
   (d) Sequential retrieval of slant column densities of NO_2 and interferring species (H_2O and CHOCHO);
   (e) Estimation of uncertainties in the retrieved values using the curvature of the chi-squared surface around the retrieved point;
2. Stable solar irradiances are now calculated from the current or previous month's OMI measurements of the solar irradiances. In the previous versions, a constant reference solar irradiance spectrum was used.

3. Improved GMI model-based monthly *a priori* NO_2 and temperature profiles [Douglass et al., 2004] replace the year-independent monthly climatologies used in version 2.1. Specific improvements include:

   (a) Resolution increased to 1 deg (latitude) x 1.25 deg (longitude);

   (b) Updated emissions inventory data;

   (c) Updated meteorological fields;

   (d) Updated chemical and photochemical reaction rates.

These improvements are described in this document, as well as in the references.

Table 2: Table of abbreviations, acronyms, and initializations (AAI) used in this document.

Abbr.	Meaning
AAI	Abbreviations, acronyms, and initializations
AMF	Air mass factor
APP	Application (production software unit)
AVDC	Aura Validation Data Center
CTM	Chemistry and Transport Model
DEM	Digital elevation model
DOAS	Differential Optical Absorption Spectroscopy
EOS	Earth Observing System
ETOPO1	Earth TOPOgraphy data product
FoV	Field of view
GMI	Global Modeling Initiative
GSFC	Goddard Space Flight Center
HDF-EOS	HDF EOS data file format
GES-DISC	Goddard Earth Sciences Data and Information Services Center
KNMI	Koningklijk Nederlands Meteorologisch Instituut
LECT	Local equator crossing time
L-1B	Level-1B (data product with calibrated radiances or irradiances)
L-2	Level-2 (data product with retrieved geophysical values)
L-2G	Gridded Level-2 (data product in grid format)
L-3	Level-3 gridded data product
NASA	National Aeronautics and Space Administration
OMI	Ozone Monitoring Instrument
RA	Row anomaly
SCD	Slant column density
SIPS	Science Investigator Processing System
CCD	Charge-coupled device
VCD	Vertical column denisty
VIS	OMI visible-wavelength detector

2 Introduction

Nitrogen oxides ($NO_x = NO + NO_2$) are species that play key roles in tropospheric and stratospheric ozone chemistry. Further, high surface level NO_2 is itself recognized to be deleterious to human health. NO and NO_2 are in quasi-steady-state in the atmosphere, and their relative concentrations depend on temperature, solar illumination, emissions, and the concentrations of other chemical species. Major sources of tropospheric NO_x include combustion, soil emissions, and lightning. While spectroscopic measurements of thermospheric, mesospheric, and upper-stratospheric NO have been made from satellite instruments, no satellite-based NO measurements have been made in the lower atmosphere. By contrast, tropospheric and stratospheric NO_2 columns are readily measured.

NO_2 column amounts are retrieved from measurements made by the Ozone Monitoring Instrument's (OMI) visible wavelength (VIS) detector in the spectral range 402–465 nm. The Level 2 (L-2) NO_2 product (OMNO2) includes stratospheric, tropospheric, and total columns.

OMI was launched on July 15, 2004, on the NASA EOS Aura satellite, which is in a sun-synchronous ascending polar orbit with a local equator crossing time (LECT) of 13:45±0:15. Science-quality data operations began on October 1, 2004.

OMI makes simultaneous measurements in a swath of width 2600 km, divided into 60 fields of view (FOVs).[1] The FOVs vary in size from $\sim 13\text{km} \times 26\text{km}$ near nadir to $\sim 40\text{km} \times 250\text{km}$ at the outermost FOVs. Figure 1 shows the relation between the OMI instrument and its viewing geometry.

2.1 Spatial coverage of OMI

Figure 2 shows the positions and sizes of these FOVs relative to the flight direction. One swath is measured every two seconds. Due to the optical characteristics of the instrument, adjacent swaths overlap considerably in

[1] There is a diversity of terminologies that are used within the EOS and OMI communities to describe an instrument's viewing area. In this document, we will use the following convention: Each measurement is made within a FOV. A set of FOVs that are measured at the same time (transverse to the orbital track–see Figure 2) is a *swath*. The set of all measurements made during a single day-side passage of the OMI instrument is a *granule*.

Some naming conventions, sometimes conflicting with ours and with each other, is, unavoidably, inherited into the NO_2 data products from various other data products and file structure specifications. Synonyms for swath include: *exposure, row, scan, scanline, and iTime*. Synonyms for FOV include: *pixel, groundpixel, scene, scan position, cross-track position, iXtrack, and row.* The term *orbit* refers to a granule. *Swath*, in the HDF-EOS5 convention, refers to a granule.

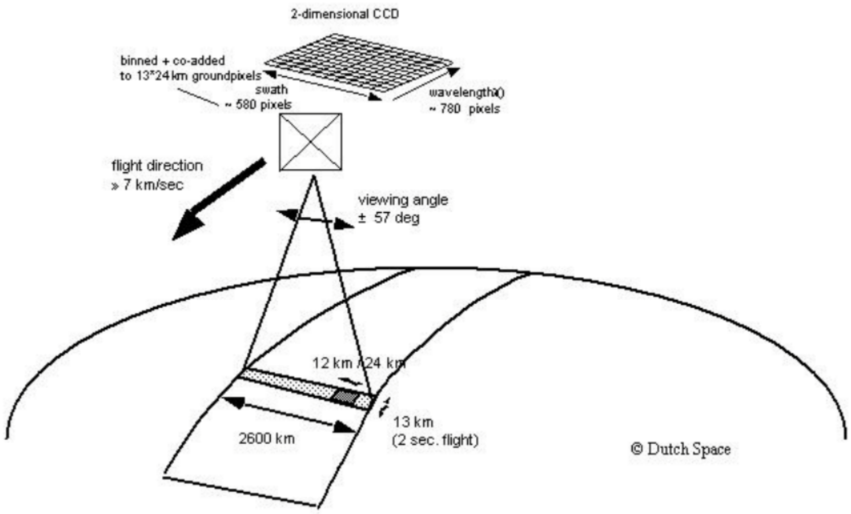


Figure 1: The OMI instrument and its viewing geometry.

their ground coverage. The width of a swath ensures that swaths from adjacent consecutive orbits are nearly contiguous at the equator and have some overlap at mid- to high-latitudes. In a single orbit, OMI measures approximately 1650 swaths from terminator to terminator. With an orbital period of 99 minutes, OMI views the entire sunlit portion of the Earth in 14–15 orbits.

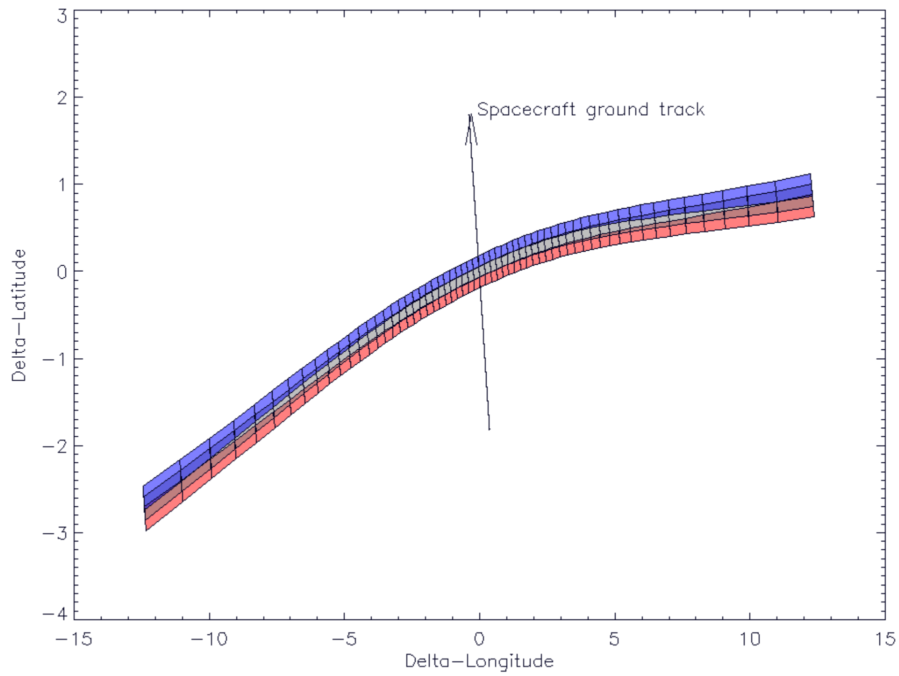


Figure 2: Geometry of the OMI FoVs near the equator. The vertical scale is exaggerated by a factor of ~ 3, relative to the horizontal scale. The colored tiles show the geometries of three successive swaths (exposures) of OMI FoVs (red, gray, and blue) near the equator. In the middle of the swath, there is very little overlap between consecutive FoVs. There is greater overlap for FoVs closer to the edge of the swath. In the outermost positions, the areal overlap between consecutive FoVs is nearly 50%.

2.2 Temporal coverage of OMI

For any position on the Earth, the OMI measurement time is generally not equal to the LECT. For near-nadir FoVs, the local overpass time is generally earlier than the LECT in the Northern Hemisphere, and later in the Southern Hemisphere. Around latitudes 50 degrees South and North, the local time of observation for near-nadir FoVs is about 1 hour later or earlier, respectively. The difference is larger off-nadir FoVs. In a swath the observational time is earlier for western FoVs and later for eastern FoVs (Fig. 3). Appendix A describes how to calculate local times for OMI observations.

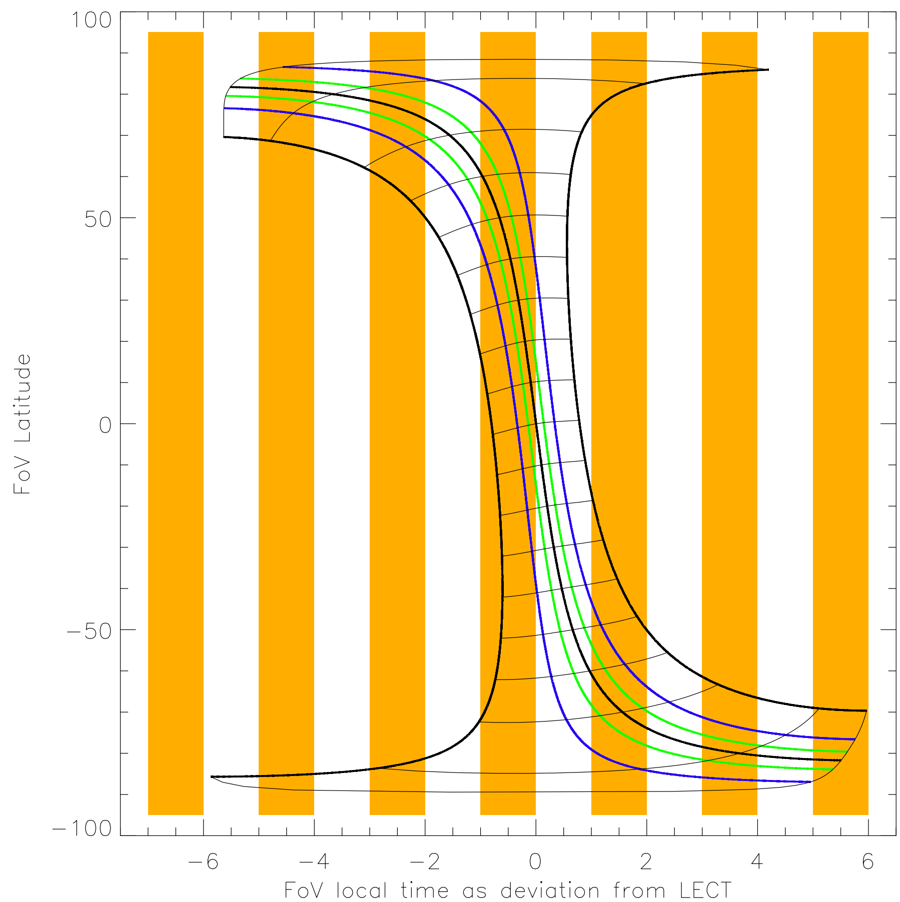


Figure 3: Deviation of local solar time (LST, "sundial time") from local equator crossing time (LECT) along the ascending leg of the OMI orbit. The local time at the subsatellite point (near scan positions 29 and 30) is shown as the thick black curve in the middle. Curves are also shown for for scan positions 0 and 59 (black), 10 and 49 (blue), and 20 and 39 (green). The nearly horizontal curves connect the FOV centers that are measured simultaneously, in a single swath. These are chosen as the times when the subsatellite point crosses latitudes $-80, -70, \cdots, +70, +80$. The slight asymmetry of the figure, between the southern and northern hemispheres is mainly due to the fact that OMI's FOVs are not arrayed symmetrically about the flight vector.

2.3 Row anomaly

Starting June 25, 2007, an anomaly began to appear in the L-1B radiances, attenuating the measured radiances in certain FoVs (53 and 54). Then, on May 11, 2008 cross-track positions 37–42 started to be affected toward the northern end of the OMI orbit. The anomaly has developed and changed over the period since. This phenomenon has been named the "row anomaly" (RA) referring to affected FoVs (rows) of the CCD detector.

Four distinct effects on the OMI radiance specta have been identified: (1) Blockage–a decrease in radiance level. It is currently assumed that this is caused by a partial blocking of the OMI viewing port; (2) Solar radiation–an increase in the radiance levels for the northern part of the orbit. It is assumed to be caused by the reflection of sunlight into the viewing port by the material blocking the port; (3) Wavelength shift–The blocking object causes an inhomogeneous illumination of the instrument's spectral slit, which induces a shift in the spectral dispersion; and (4) Radiance received from outside the nominal FoV. These effects are discussed in the web document "Background information about the Row Anomaly in OMI" (http://projects.knmi.nl/omi/research/product/rowanomaly-background.php).

The data quality for RA-affected FoVs is sufficiently poor as to prevent the retrieval of NO_2 column amounts. In version 3.0, we have abandoned the retrieval calculations of the VCDs (`ColumnAmountNO2`, *etc.*), and inserted fill-values into those fields where the RA has been identified. We found that, for certain epochs, the RA scheme implemented in the L-1B APP gives false-negatives, not flagging some clearly-affected FoVs adjacent to flagged FoVs. We have implemented additional flagging in the OMNO2 and OMNO2G data products in those cases.

Row anomaly information is available in the `XTrackAnomalyFlags` data field. In the OMNO2 data product, the content of this field reflects our additional flagging, so it is not identical to the so-named field in other data products.

2.4 Zoom mode

The OMI instrument has a number of operating configurations, including *global* measurements (the ordinary measurement), *spatial-zoom*, *spectral-zoom*, and a variety of calibration modes. The mode of operation for any measurement is indicated by the `InstrumentConfigurationID` field. The retrieval code has not been optimized for use with either of the zoom-measurement modes. For that reason, the calculation of the vertical column densities (`ColumnAmountNO2`, for example) has been abandoned when the instrument is not in global measurement mode, and a fill-value will be found in each of these data fields.

There are some instances when a set of 14 or more consecutive orbits have made measurements in zoom mode. Users will find that there are no valid data in the files for these orbits.

2.5 Data quality

The algorithms used to produce L-2 data products are very complex (see Figure 4), and the incoming data from the satellite can be noisy—any individual measurement may be anomalous. We have gone to great lengths to automatically recognize anomalous measurements. Many anomalies may be sufficiently severe that the calculation is abandoned, and the derived quantities are assigned a fill-value. Less severe anomalies may not demand abandoning the calculation.

We provide a summary quality flag–a single bit that may be interrogated to select data. This is the least-significant bit of the field `VcdQualityFlags` (See Section 4.3). We *strongly* recommend that most users select *only* data for which the least-significant bit of `VcdQualityFlags` is zero, indicating good data. This may be done using a bitwise logical *and* operation on `VcdQualityFlags` and the integer '1'. For example, in FORTRAN,

```
goodData = ( IAND( VcdQualityFlags , 1 ) .EQ. 0 )
```

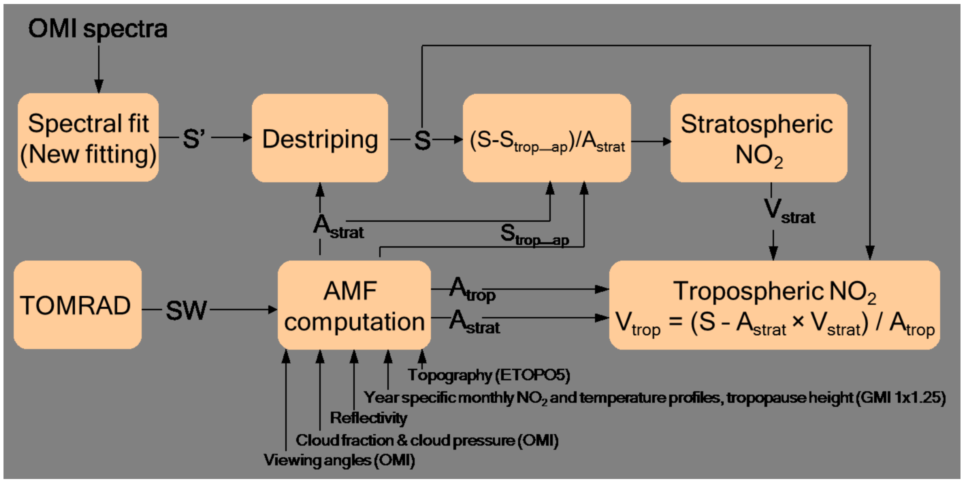


Figure 4: Schematic description of the OMI NO_2 processing algorithm. S variables represent slant column densities; A variables represent air mass factors (AMF). V variables represent vertical column densities. SW indicates scattering weight, which was computed using the radiative transfer program TOMRAD.

3 Algorithm description

The OMI Level 1b data product contains calibrated earthshine radiance spectra $\mathbf{I}$ for each FOV. Earthshine radiances are divided by the solar irradiance spectrum $\mathbf{F}$ to give a normalized spectrum $\mathbf{R} = \mathbf{I}/\mathbf{F}$. The trace gas ($NO_2$, H_2O, CHOCHO) slant column amounts are retrieved from the normalized spectrum. The slant column amounts are combined with stratospheric and tropospheric air mass factors to obtain vertical columns.

Figure 4 shows schematically the data flow through the algorithm. The individual steps are described in more detail in the following subsections.

3.1 Solar spectral irradiance

OMI makes daily solar spectral irradiance measurements that are processed and archived. The original intent was that, in processing an orbital granule into any L-2 product, the most recent solar irradiance spectra, acquired within the preceding 24 hours, would be used. Soon after operations began, pronounced irregular patterns across a swath appeared in retrieved quantities in all OMI L-2 products; these patterns were relatively consistent along-track, and so were dubbed "striping." The stripes changed from orbit to orbit. The use of a static solar reference spectrum ameliorated much of the calibration-induced striping. However, as we have learned more about the sensitivity of OMI to solar variations, and indeed the scale of those variations, we have found it necessary, starting with version 3.0, to use monthly irradiances that are computed as a separate data product. These irradiances are carefully determined, statistically, from a month's irradiance measurements. (See below.) A destriping step is still used in the OMNO2 processing, though it has generally a smaller effect, and we are accordingly more confident that substantial biases are not introduced by that step.

The OMI NO_2 slant column retrieval algorithm starts from radiances, normalized to monthly-averaged solar irradiances (Section 3.2). We choose the monthly averages as a compromise between the required high S/N of the solar data, and the need to account for long-term instrumental drifts, as well as for the solar variability, which is quite noticeable in the S/N $\gtrsim$ 1000 solar spectra [Marcheko and DeLand, 2014].

To produce the solar monthly averages, we correct the daily OMI solar irradiances for the time-varying Sun-Earth distance. At each wavelength of the 402–465 nm domain used in the NO_2 retrievals we assess stability of the wavelength registration, linearly interpolating the spectra with deviations exceeding 0.002 nm to a common wavelength grid. At each wavelength the daily irradiances are searched for $\pm 1.5\sigma$ outliers. These are substituted with a reference spectrum comprised of an unweighted 3-month (January–March 2005) average of measured solar spectra, adjusted for instrumental drifts and solar variability. The wavelength-corrected, cleaned daily spectra are then directly (no weights) averaged into monthly solar means.

3.2 Slant column retrieval

NO_2 slant column densities are computed using a completely new algorithm [Marchenko et al., 2015] that improves the trace gas retrieval by increasing the accuracy of the wavelength registration between radiance and irradiance spectra. The wavelength registration procedure relies on the structure of the Ring effect spectrum (rotational Raman scattering), whose amplitude in the spectral region of interest is much greater than spectral features of the trace gases. Wavelength calibrations are performed independently in each of seven spectral windows inside the window 402–465 nm. With this calibration, the dominant Ring feature is subtracted from $\mathbf{R}$, and three trace gases, NO_2, H_2O, and CHOCHO are successively estimated by fitting to the resulting spectrum to the laboratory-measured spectra in a variation of the Differential Optical Absorption Spectroscopy (DOAS) method. A further step corrects for undersampling by the OMI instrument [Chance et al., 2005]. With the undersampling correction in hand, the entire process of wavelength calibration followed by successive trace gas retrieval is repeated. The result of the spectral fit is a slant column density `SlantColumnAmountNO2`.

3.3 AMF calculation

The air mass factor (AMF) is defined as the ratio of the measured slant column density S to the vertical column density V. AMFs depend upon a number of parameters including optical geometry (solar and viewing azimuth and zenith angles), surface reflectivity, cloud pressure and fraction, and the shape of the NO_2 vertical profile. The AMFs are computed from the scattering weights (Section 4.3) and a monthly mean climatology of NO_2 profile shapes constructed from the Global Modeling Initiative (GMI) Chemistry and Transport Model (CTM) simulation, with a horizontal resolution of 1.25° longitude ×1.0° latitude. The simulation is based on yearly-varying emissions, as discussed in Strode et al. [2015]. Model profiles are generated in 15 minute time steps. The profiles used for the AMFs are the averages of the profiles at timesteps from 13:00 to 14:00, local time. The scattering weights are corrected for the atmospheric temperature profile, which compensates for the fact that the SCD retrieval is done assuming a constant NO_2 temperature (220 K).

Stratospheric and tropospheric AMFs are calculated, (A_{strat} and A_{trop}) separated at the climatological GEOS-5 monthly tropopause pressure.

While stratospheric NO_2 retrieval is nearly insensitive to NO_2 profile shape assumption, tropospheric NO_2 retrieval is sensitive to the NO_2 profile shape, temperature profile, and surface reflectivity. Use of monthly NO_2 profile shapes captures the seasonal variation in NO_2 profiles [Lamsal et al., 2010]. The present version (3.0) uses annual monthly profiles from 2004 to 2014. For dates starting in 2015, the 2014 monthly profiles are used.

The method of AMF calculation is similar to that described by Palmer et al. [2001]. For each FoV, AMFs are computed for clear ($\text{AMF}_{\text{clear}}$) and cloudy ($\text{AMF}_{\text{cloud}}$) conditions. The AMF of a partially clouded scene is calculated by:

$$\text{AMF} = (1 - f_r) \cdot \text{AMF}_{\text{clear}} + f_r \cdot \text{AMF}_{\text{cloud}} \quad (1)$$

where f_r is the cloud radiance fraction (CRF), *i.e.* the fraction of the measured radiation that comes from clouds and scattering aerosols. The CRF is computed from the effective cloud fraction f_c (from the independent OMCLDO2 data product), using tables constructed from radiative transfer calculations, as part of the OMNO2A algorithm. Note that the CRF is usually larger than f_c, since the clouds are usually much brighter than the surrounding atmosphere at 440 nm. $\text{AMF}_{\text{clear}}$ is calculated assuming a Lambertian surface of reflectivity R_s at pressure P_s, determined from a digital elevation model (DEM; ETOPO1). $\text{AMF}_{\text{cloud}}$ is calculated assuming a Lambertian surface of reflectivity 0.8 at cloud pressure P_c. R_s and P_s are obtained from a climatological database. P_c and f_c are obtained from the OMCLDO2 product. Please refer to the OMCLDO2 Readme file for relevant details.

3.4 Destriping

The measured NO_2 SCDs are corrected for an instrumental artifact that varies across the orbital track and results in the appearance of "stripes" along the track. The severity of this artifact was greatly diminished, in previous versions, by the use of a static solar spectrum. Version 3.0 improves the product further by using statistically adjusted monthly median solar irradiances (see Section 3.1). The destriping algorithm computes the mean cross-track biases using measurements obtained at latitudes between 30S and 5N and from orbits within 2 orbits of target orbit. These are essentially a set of 60 correction constants, one for each cross-track position, that are subtracted from the measured VCDs to calculate the destriped SCD field, `SlantColumnAmountNO2Destriped` (see Section 4.3). Although the uncorrected SCDs (`SlantColumnAmountNO2`) are also stored in the Level 2 files, we do not use them to calculate the VCDs.

3.5 Stratosphere-troposphere separation

The stratospheric and tropospheric column amounts are retrieved separately under the assumption that the two are largely independent. The stratospheric field is computed first, beginning with creation of a gridded global field $V_{\text{init}} = S/\text{AMF}_{\text{strat}}$ values, assembled from data taken within ± 7 orbits of the target orbit. An *a priori* estimate of the tropospheric contribution to this field, based on a monthly GMI model climatology and cloud measurements, is subtracted, and grid cells where this contribution exceeds 0.3×10^{15} molecules cm^{-2} are masked. Masking ensures that the model contribution to the retrieval is minimal. Note that not all highly polluted areas will be masked in this procedure, since clouds may already hide the tropospheric NO_2 from OMI in those regions. A three-step (interpolation, filtering, and smoothing) algorithm is then applied to fill in the masked regions and data gaps, and to remove residual tropospheric contamination. The resulting stratospheric vertical column field V_{strat} is converted to a slant column field using $\text{AMF}_{\text{strat}}$, and subtracted from S to give the tropospheric slant column. Dividing this by the tropospheric air mass factor AMF_{trop} gives the tropospheric vertical column V_{trop}. For details see Bucsela et al. [2013].

4 Level-2 Data Product

4.1 File name

OMNO2 L-2 files are written in HDF-EOS version 5 (HDF-EOS5) format and have the following naming convention [Craig et al., 2006, Claas, 2011]:

```
<InstrumentID>_<DataType>_<DataID>_<Version>.<Suffix>,
```

where

```
<DataID> = <ObservationDateTime>-o<Orbit#>
```

and

```
<Version> = v<Collection#>-<ProductionDateTime>
```

Below is an example of an OMNO2 L2 file name:

```
OMI-Aura_L2-OMNO2_2011m1010t2318-o38499_v003-2011m1011t154524.he5
```

where:

<InstrumentID>	=	OMI-Aura
<DataType>	=	L2-OMNO2
<ObservationDateTime>	=	2011m1010t2318
<Orbit#>	=	38499
<Collection#>	=	003
<ProductionDateTime>	=	2011m1011t154524
<Suffix>	=	he5

The observation time is stated to the minute (4 digits); the processing time is stated to the second (6 digits).

4.2 File organization

The HDF-EOS5 file structure is shown in Figure 5.

As HDF-EOS5 files, OMNO2 L-2 files contain a single swath, called `ColumnAmountNO2`, composed of a `Geolocation Fields` group and a `Data Fields` group. This section briefly describes the more commonly-used data fields. A complete list of the fields and metadata information contained in the OMNO2 files can be found in Celarier et al. [2016].

4.3 Data description

Two kinds of data fields are found in the file: product data, and flags. While most product data fields are of a floating-point ("real") type, some, such as `CloudFraction`

Figure 5: OMNO2 HDF-EOS5 file structure.

have been stored as integers to make the file a bit smaller. The fields have field-level metadata which characterize the values contained in the data fields. These include the fill-values that are used when no meaningful data are available, and a scale factor and offset. These are usually 1 and 0, respectively, indicating that the values have not been modified. However, `CloudFraction` is one exception, since the integer values stored are 1000 times the actual value: Its scale factor is 0.001 The field `TerrainReflectivity` is similarly scaled.

Flag fields may have 8, 16, 32, or 64 bits per word, stored as unsigned integer values (one word per FOV or per swath, as appropriate), containing a collection of bits that each indicate processing conditions that should be taken as warnings or errors, or may indicate which path was taken through one of the algorithms, or may indicate why some data field(s) have been assigned fill values. The meanings of single bits, and groups of bits, for each flag field are found in Celarier et al. [2016].

The following paragraphs describe briefly the fields that are of the greatest interest to most end-users of the data product. A complete list of data fields is in Table 7.

SlantColumnAmountNO2Destriped and **SlantColumnAmountNO2Std**: Retrieved slant column density (SCD) S and its uncertainty. S is the retrieved total areal density of NO_2 molecules along the effective optical path from the sun into the atmosphere, and then toward the satellite. This is calculated from the measured Earthshine radiance and solar irradiance using a variant of the DOAS algorithm (see section 3), with an NO_2 cross section measured at 220 K. Variations that are due to calibration differences between the detector cells have been removed using the destriping procedure described in Section 3.4. The units are molecules cm^{-2}.

ColumnAmountNO2Strat and **ColumnAmountNO2StratStd**: Estimates of the stratospheric vertical column density (VCD), V_{strat}, derived from S, and its uncertainty. The units are molecules cm^{-2}.

ColumnAmountNO2Trop and **ColumnAmountNO2TropStd**: Estimates of the tropospheric vertical column density, V_{trop}, derived from S, and its uncertainty. The units are molecules cm^{-2}.

ColumnAmountNO2 and **ColumnAmountNO2Std**: Estimates of the total (i.e., $V = V_{\text{strat}} + V_{\text{trop}}$) vertical column density and its uncertainty. The units are molecules cm^{-2}.

ScatteringWeight: Vector **A** [no units] that describes the relationship between slant column density, S_i, and the vertical column density, V_i, for each atmospheric layer i:

$$S = \sum_i S_i \approx \sum A_i \cdot V_i \qquad (2)$$

A is relatively insensitive (within $\sim$ 20%) to the wavelength within the spectral region used in OMNO2, so only a single value, representative of the entire spectral fitting window, is provided. **A** is a function of the optical geometry (solar and viewing azimuth and zenith angles), surface reflectivity, and cloud pressure and cloud fraction, and contains a correction for the temperature dependence of the NO_2 cross section. The scattering weights are stored as a 3-dimensional array with dimensions (pressure levels, across track, along track; *e.g.* [35,60,1644]). The grid of pressure levels is available as the data field `ScatteringWtPressure`.

Partial slant column (*e.g.* tropospheric) densities may be computed from Eq. (2) using ranges of i falling within the partial column, and V_i values derived from models. The partial column Air-Mass Factor (AMF) (*e.g.* AMFtrop, Section 3.3) can be obtained by dividing Eq. (2) by the corresponding partial vertical column (*e.g.* V_{trop}). Methods for comparing OMI columns with external datasets may be found in Bucsela et al. [2008], Lamsal et al. [2014], and references therein.

XtrackQualityFlags: The cross-track quality flags indicate specific likely problems with the radiance measurements, due to the row anomaly (Section 2.3). As a general rule, for files with measurements after June 2007, one should not use data where the `XtrackQualityFlags` field is nonzero. For these FOVs, the current data product version, the column amount fields are set to their fill values. However, before this time, the `XtrackQualityFlags` words are set to a fill value. Thus, the user should only use Level 2 data where `XtrackQualityFlags` is equal to zero, *or* equal to the fill value. The fill value can be found in each field's metadata.

vcdQualityFlag: This variable contains quality assurance information for the tropospheric vertical column. The least significant bit is the **summary quality**

flag. We recommend that users only use data for which this bit is zero (*i.e.*, `vcdQualityFlag` is an even integer).

4.4 Limitations

As with all remote sensing data sets, there are subtleties in the OMNO2 data that are due to geophysics, instrumental measurements, and the retrieval algorithm. Users of the data are encouraged to communicate directly with members of the OMI NO_2 algorithm team. We also encourage those using the data to read Bucsela et al. [2013] and Marchenko et al. [2015], which describe the algorithm in detail.

Particular attention should be paid to the various data quality flags. For most users, the Summary Quality Flag (least significant bit of the `vcdQualityFlags` data field) should suffice. In row-anomaly-affected FoVs, the column amount fields have been set to their respective fill values, so `XTrackQualityFlags` does not need to be explicitly checked. In certain periods of time, using these flags will result in up to 50% field-of-view rejection rate.

While features inherent to the stratospheric NO_2 field are relatively large, compared to the geographical extent of OMI's larger (far-off-nadir) FoVs, many local features in tropospheric fields are smaller than OMI FoVs. This may lead to a negative bias in the column amounts when there is a local maximum within the FoV. This should be a consideration when computing statistics from multiple measurements. The retrieval algorithm permits the values of any of the columns to be negative. In particular, small-magnitude negative values are not uncommon in areas that are generally unpolluted (*e.g.* over open oceans). When computing statistics, it is important to include all valid measurements, regardless of their sign, in order to avoid biases.

Studies (*e.g.* trend analyses) based on periods of time where some of the data are heavily flagged or filled should be sampled in such a way that the contribution from each scan position has similar weight throughout the period of interest. For example, in a time-series analysis of data over a time-span that includes periods of RA-affected and periods of non-RA-affected measurements, the non-RA periods should be sampled to include only those cross-track positions that are unflagged in the RA period.

OMI has a number of measurement modes. Besides the normal "global" mode, it has two "zoom" modes. Zoom mode measurements are indicated by the field `InstrumentConfigurationID` having a value > 7. This version of the retrieval algorithm does not perform well in either of the zoom modes. Therefore, when the instrument is operating in a zoom mode, no NO_2 vertical amounts are calculated. This occasionally results in entire orbital granules having nothing but fill-values for the NO_2 column fields.

5 The Level-2 gridded NO_2 product, OMNO2G

The Level-2 HDF-EOS5 files, described in Section 4.3, are used to create Level-2-gridded, daily data products, called OMNO2G. These are also HDF-EOS5 files, but are Grid type, rather than Swath type files. Each $0.25° \times 0.25°$ geographical grid cell can be thought of as containing a "stack" of up to 15 L-2 FoVs' data collocated with the grid cell. In practice, only up to ~ 6 are populated. The OMNO2G data product can be useful for considering L-2 data within a geographic area of interest. It was originally conceived as a "global overpass" data set. It does have the advantage of containing a geographically sorted list of L-2 FoVs, which may be more convenient for users interested in regional NO_2 fields.

Since only as many as 15 L-2 fov s are identified with a grid cell, there may be some selection: greater priority is given to FoVs having the shortest optical path length (defined as $\sec\theta + \sec\theta_\circ$, where θ is the viewing zenith angle, and $\theta_\circ$ is the solar zenith angle). The user should be aware that the identification of a L-2 FoV with a grid cell is based entirely on the location of the FoV center. Since the grid array has a spatial resolution of 0.25°, and many of the OMI fields-of-view are considerably larger than that, it is a good idea to examine data that are identified with a larger region than the actual region of interest.

5.1 File name

The file name for the OMNO2G files is of the form:

```
OMI-Aura_L2G-OMNO2G_<ObservationDate>_v003-<ProductionDate>.he5
```

An example is:

```
OMI-Aura_L2G-OMNO2G_2013m0102_v003-2013m0103t183921.he5
```

5.2 File structure

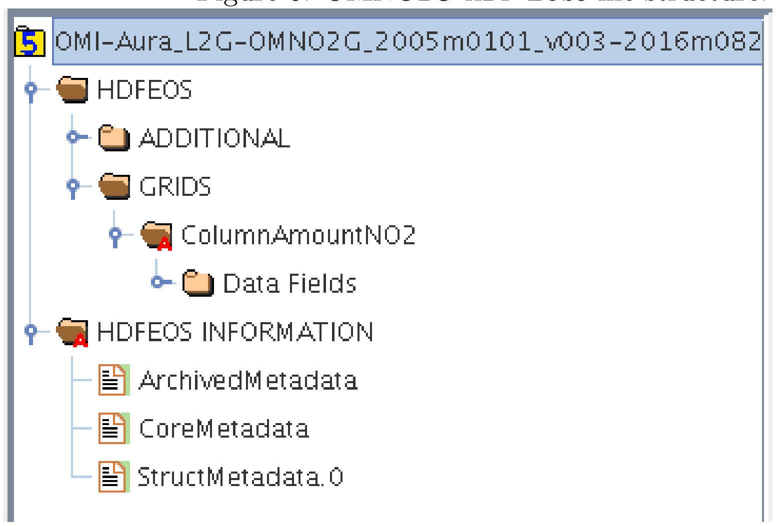
The structure of the HDF-EOS5 data file is shown in Figure 6. There are 38 data sets within the `Data Fields` group, which are selected from the L-2 data. Table 7 lists all the fields.

Each data field has dimensions [1440 , 720 , 15] (number of cells in the longitude direction, number of cells in the latitude direction, and maximum L-2 FoVs identified with each cell, respectively). Unpopulated elements in the data field are assigned a fill value.

5.3 Data fields

The data fields are listed in Table 7. While most of the fields' names and data values are inherited from the OMNO2 data product, there are several that are unique to the OMNO2G. We describe those here.

Figure 6: OMNO2G HDF-EOS5 file structure.



OrbitNumber Since the OMNO2G compiles data from multiple orbits into a single daily file, the data in the stack are may be associated with different orbits. This field identifies the orbit.

LineNumber The swath (exposure) number in the along-track direction (0-based).

SceneNumber The cross-track position of the FoV. (0-based)

NumberOfCandidateScenes The number of populated members in the stack. The maximum is 15. Typical values range from 0 to 6.

PathLength The length of the optical path; it is also the geometric air mass factor. It is equal to $\sec\theta_o + \sec\theta$, where θ_o is the solar zenith angle and θ is the viewing zenith angle.

5.4 Limitations

Since the L-2 data are copied directly into the OMNO2G data product, the general quality of the data is the same. (See Section 4.4.) For some purposes, in some geographical regions (*e.g.* in polar regions), more than 15 L-2 FoVs may have their centers land in a particular cell, and some L-2 data, whose optical path lengths are longer than the others, may be excluded. This should happen rarely, but may lead to slight shifts in statistical measures.

Since the identification of a grid cell with a L-2 FoV is based solely on the location of its center, some FoVs identified with nearby grid cells may be relevant to a particular grid cell.

In the current version of OMNO2G, the FoV corners (from the product OMPIXCOR) are not copied from the L-2 files. Any work that involved detailed knowledge of the L-2 FoV geometries will have to be done using either the L-2 data product (OMNO2) or the OMPIXCOR data product.

6 The Level-3 gridded NO_2 product, OMNO2d

The L-2 HDF-EOS5 files, described in Section 4.3 are used to create L-3 daily data products, called OMNO2d. These are also HDF-EOS5 files, but are Grid type, rather than Swath type files. In the archived data product, a day's worth of L-2 data (usually 14 or 15 orbits) are mapped into a single $0.25° \times 0.25°$ latitude-longitude grid. The parameters specifying the grid cell locations are available in the metadata included in each file. Each file contains five (5) grid fields: `ColumnAmountNO2`, `ColumnAmountNO2CloudScreened`, `ColumnAmountNO2Trop`, `ColumnAmountNO2TropCloudScreened`, and `Weight`. (See Table 7.)

In each of the first four of these fields, the value given in any grid cell is an area-weighted average of the values of the corresponding field (`ColumnAmountNO2` or `ColumnAmountNO2Trop`) in all the L-2 FOVs that have any overlap at all with that grid cell. See the OMPIXCOR Readme file for more information. The weighting scheme is described below. The L-3 data product is available from the Goddard Earth Sciences Data and Information Services Center (GES-DISC). See Section 10 for details.

6.1 File name

The names of the OMNO2d files are of the form:

```
OMI-Aura_L3-OMNO2d_<ObservationDate>_v003-<ProductionDate>.he5
```

An example is:

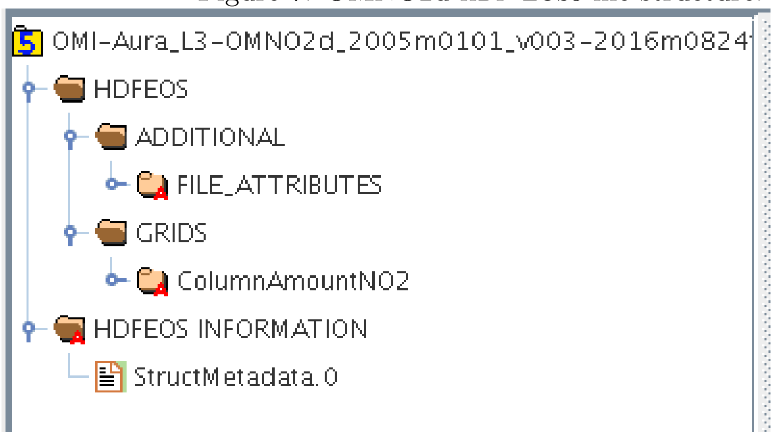
```
OMI-Aura_L3-OMNO2d_2007m0915_v003-2012m1126t105634.he5.
```

6.2 File structure

The structure of the HDF-EOS5 data file is shown in Figure 7. Metadata are found in four places:

1. Structural metadata are in `/HDFEOS INFORMATION/StructMetadata.0`;
2. Metadata concerning the source data are found in `/HDFEOS/ADDITIONAL/FILE_ATTRIBUTES`;
3. The grid metadata are in group attributes of the group `/HDFEOS/GRIDS/ColumnAmountNO2`;
4. Metadata concerning individual fields is attached to the grid fields themselves.

Figure 7: OMNO2d HDF-EOS5 file structure.



6.3 Data fields

The data fields contain the gridded data. The first grid cell (the one with the smallest indices) has edges at 180° West longitude and 90° South latitude. Grid cells that did not have any overlapping L-2 FoVs among the input files are assigned a fill value ($-2.^{100} \simeq -1.26765\times10^{30}$). The data are in units of molecules cm^{-2}. All the NO_2 data fields are produced by first screening the L-2 data, and then calculating the weighted average of the remaining data. The screening criteria are listed in Table 4.

Table 4: Criteria used to screen OMNO2 data for use in generating OMNO2d data product.

Field	"Pass" criterion
SolarZenithAngle	$< 85°$
TerrainReflectivity	$< 30\%$
CloudFraction	$< 30\%$ (For cloud-screened fields)
CloudFraction	No filter (For other fields)
XTrackQualityFlags	0 or 255
vcdQualityFlags	Asceding orbit; Summary flags not set

The weighted averages are computed as follows: For each grid cell (j) and each L-2 FoV (i), the area of overlap (Q_{ij} = area of overlap ÷ area of grid cell) is computed, and the area of the FoV A_i is known. The weight is linear with A_i:

$$w_{A_i} = 1 - (A_i - A_{\min})/A_{\max} \tag{3}$$

(larger area, smaller weight) , and is proportional to the area of overlap (larger overlap, larger weight.) The weight for FoV i and cell j is

$$w_{ij} = w_{A_i} \cdot Q_{ij}. \tag{4}$$

The total of all weights for cell j, w_j , is stored in the data field `Weight`. This can be used to combine gridded data from multiple L-3 files and geographical regions in order to rapidly compute spatial or temporal averages. Indexing the relevant data sets by k, compute V_j:

$$V_j = \frac{\sum_k w_{kj} V_{kj}}{\sum_k w_{kj}} \tag{5}$$

6.4 Limitations

While the L-3 data product can be used to assess the daily NO_2 column densities (or, when combined as described above, for longer time periods), it is important to remember that the values in the grid cells are weighted averages of a number of OMI measurements, and the value in a cell may not correspond to any one actual measurement.

Because the 8–10 OMI FoVs farthest from nadir are quite large (see Figure 2), their contribution to the weighted average in a grid cell may be affected by actual NO_2 columns some distance away from the cell. This is particularly important when looking at daily L-3 data, as, especially in the tropics, some grid cells may have contributions from only the OMI swath edge FoVs, while others have contributions from only the smaller, near-nadir FoVs. The natural spatial resolution of the former is coarser than the grid cells, while the spatial resolution of the latter is comparable to the grid cell size. To compare different small areas, one should consider the Weight field values for each. The weights of better-characterized grid cells will tend to be larger than those of less-well-characterized grid cells. This is also a consideration when constructing time-series for a set of grid cells: Because of Aura's precession relative to the fixed geographical (latitude-longitude) grid, a chosen grid cell will be under large OMI FoVs on some days, and under small ones on other days. One should especially look at the weights if one finds an apparent spatial or temporal periodicity in the NO_2 columns.

The product development team has chosen a cloud screening criterion of the effective cloud fraction $f_c < 0.30$ (see Table 4) for the cloud-screened variables, which reflects a compromise between data quality and quantity.

7 Software versions

This document applies to the public release of the OMI L-2 NO_2 data, product version 3.0, archived as collection 3 and released in August 2016. The L-2 algorithm is divided into four processes, each performed by a separate application. The end result is the creation of the OMNO2 L-2 data product from the OMI Level L-1B product. The L-0 to L-1B processing version is designated "Collection 3". This is not to be confused with OMNO2 version 3.0.

The software versions used to produce product version 3.0 are listed in Table 5.

Table 5: Version numbers of data products and the applications (Apps) that create them.

Data product	Product version	App version
OMNO2	3.0	2.0.4.00
OMNO2G	3.0.0	1.3.0
OMNO2d	3.0.0	1.0.5
OMNO2SCD		0.1.7.00
OMNO2B		1.2.1.0
OMNO2A	1.2.3.1	1.2.3.1
OMCLDO2	1.2.3.5	1.2.3.5

8 Data quality

The quality of the data in this release has been established by consistency checks with previous version (v2.1), which was extensively evaluated [Lamsal et al., 2014, Bucsela et al., 2013]. Some of our preliminary works are presented in Marchenko et al. [2015]. Our validation effort using other independent measurements and campaign data from ground-, aircraft-, and satellite-based instruments is ongoing.

The fitting error in the NO_2 slant column is estimated to be $0.3 - 1 \times 10^{15}$ molecules cm^{-2}. Preliminary comparisons of the retrieved stratospheric monthly zonal mean NO_2 columns show that they generally have decreased by $< 10 - 40\%$ relative to the version 2.1 retrieval [Marchenko et al., 2015]. The seasonal variation of OMI stratospheric NO_2 agrees with the NASA GSFC GMI chemical transport model. A document detailing validation with other ground-based and satellite datasets is in preparation.

The stratosphere-troposphere separation algorithm uses modeled atmospheric profiles. One consequence of this is that, in relatively clean regions (*e.g.* over the open ocean), the tropospheric NO_2 column is essentially model-driven, as there is no separable tropospheric column information in the slant column denisity.

Though one should expect the probability density function (PDF) of the imputed tropospheric column to be very similar to that of the model's PDF, it is found to be much wider (giving rise, for example, to a great number of retrieved negative values), and with a median that is up to 50% smaller ($< 10^{14}cm^{-2}$) than that of the model's PDF for the same region. This arises from the way the retrieved SCDs constrain the derived stratosphere. This systematic bias of the retrived tropospheric column, relative to the model tropospheric column, holds for regions identified as "clean" in the algorithm, and does not necessarily imply that the estimated tropospheric columns are biased in other regions.

9 Known issues

The uncertainty estimate fields listed below are currently being revised, and should not be used for data quality assessments.

```
SlantColumnAmountNO2Std
SlantColumnAmountH2OStd
SlantColumnAmountCHOCHOStd
ColumnAmountNO2Std
ColumnAmountNO2StratStd
ColumnAmountNO2TropStd
AmfStratStd
AmfTropStd
```

10 Product availability

The OMNO2 product is archived and distributed from the Goddard Earth Sciences Data & Information Services center (GES-DISC). The files can be directly downloaded from the GES-DISC Mirador site which provides parameters and spatial subset capabilities. OMI products are written in HDF-EOS5 format. GES-DISC also provides a list of tools that read HDF-EOS5 data files

In order to download GES-DISC data via browser window, or from the command line, or via desktop applications, you must (1) register with Earthdata Login and (2) authorize NASA GES-DISC Data Access. See the first two items below.

The following is a list of data sources and resources related to the OMNO2 data.

To register with Earthdata Login (step 1):
https://wiki.earthdata.nasa.gov/display/EL/How+To+Register+With+Earthdata+Login

To authorize NASA GES-DISC Data Access (step 2):
http://disc.sci.gsfc.nasa.gov/registration/authorizing-gesdisc-data-access-in-earthdata_login

OMNO2 data:
http://disc.sci.gsfc.nasa.gov/datacollection/OMNO2_003.html

OMNO2G data:
http://disc.sci.gsfc.nasa.gov/datacollection/OMNO2G_003.html

OMNO2d data:
http://disc.sci.gsfc.nasa.gov/datacollection/OMNO2d_003.html

Station overpass data:
http://avdc.gsfc.nasa.gov/pub/most_popular/overpass/OMI/OMNO2/

OMNO2d images:
http://avdc.gsfc.nasa.gov/

OMNO2 Readme (also covers OMNO2G and OMNO2d):
http://aura.gesdisc.eosdis.nasa.gov/data/Aura_OMI_Level2/OMNO2.003/doc/README.OMNO2.pdf

OMNO2 File description:
http://disc.sci.gsfc.nasa.gov/Aura/data-holdings/OMI/documents/v003/OMNO2_v3.0_data_product_specification.pdf

OMI Data User's Guide:
http://disc.sci.gsfc.nasa.gov/Aura/additional/documentation/README.OMI_DUG.pdf

OMI FoV corners:
http://disc.sci.gsfc.nasa.gov//datacollection/OMPIXCOR_003

GES-DISC-hosted tools for reading HDF-EOS5 files:
http://disc.sci.gsfc.nasa.gov/Aura/additional/tools.shtml

GES-DISC-hosted recipe for downloading data with wget:

http://disc.sci.gsfc.nasa.gov/recipes/?q=recipes/How-to-Download-Data-Files-from-HTTP-Service-with-wget

GES-DISC-hosted other recipes:
http://disc.sci.gsfc.nasa.gov/recipes/?q=recipe-cookbook

11 Reporting problems and requesting information

To report problems, or pose questions and comments related to the OMNO2 algorithm, data quality, and file structure, please sends electronic mail to the OMI NO_2 algorithm team: omno2@ltpmail.gsfc.nasa.gov. Additional questions may be directed to the principal point of contact for OMNO2: Nickolay.A.Krotkov@nasa.gov

Table 7: Fields available in the three OMI NO_2 data sets. D indicates fields in the *Data Fields* group; G indicates fields in the *Geolocation Fields* group.

Field	OMNO2	OMNO2G	OMNO2d
AMFQualityFlags	D		
AlgorithmFlags	D		
AmfStrat	D		
AmfStratClear	D		
AmfStratCloudy	D		
AmfStratStd	D		
AmfTrop	D		
AmfTropClear	D		
AmfTropCloudy	D		
AmfTropStd	D		
CloudFraction	D	D	
CloudFractionStd	D	D	
CloudPressure	D	D	
CloudPressureStd	D	D	
CloudRadianceFraction	D	D	
ColumnAmountNO2	D	D	D
ColumnAmountNO2CloudScreened			D
ColumnAmountNO2Std	D	D	
ColumnAmountNO2Strat	D	D	
ColumnAmountNO2StratStd	D	D	
ColumnAmountNO2Trop	D	D	D
ColumnAmountNO2TropCloudScreened			D
ColumnAmountNO2TropStd	D	D	
FoV75Area	G		
FoV75CornerLatitude	G		
FoV75CornerLongitude	G		
GroundPixelQualityFlags	G		
InstrumentConfigurationId	D	D	
Latitude	G	D	
LineNumber		D	
Longitude	G	D	
MeasurementQualityFlags	D	D	
NumberOfCandidateScenes		D	
OMNO2SCD_algoFlags	D		
OMNO2SCD_algoxFlags	D		
OMNO2SCD_procFlags	D		
OMNO2SCD_radFlags	D		

Continued...

Table 7, continued.

Field	OMNO2	OMNO2G	OMNO2d
OMNO2SCD_scdFlags	D		
OMNO2SCD_wvlnFlags	D		
OrbitNumber		D	
OrbitPhase	G		
PathLength		D	
ScatteringWeight	D		
ScatteringWtPressure	D		
ScdApStrat	D		
ScdApTrop	D		
SceneNumber		D	
SlantColumnAmountCHOCHO	D		
SlantColumnAmountCHOCHOStd	D		
SlantColumnAmountH2O	D		
SlantColumnAmountH2OStd	D		
SlantColumnAmountNO2	D	D	
SlantColumnAmountNO2Destriped	D	D	
SlantColumnAmountNO2Std	D	D	
SmallPixelRadiance	D		
SmallPixelRadiancePointer	D		
SolarAzimuthAngle	G	D	
SolarZenithAngle	G	D	
SpacecraftAltitude	G	D	
SpacecraftLatitude	G	D	
SpacecraftLongitude	G	D	
TerrainHeight	D		
TerrainPressure	D	D	
TerrainReflectivity	D	D	
Time	G	D	
TropopausePressure	D	D	
VcdApBelowCloud	D		
VcdApStrat	D		
VcdApTrop	D		
VcdQualityFlags	D	D	
ViewingAzimuthAngle	G	D	
ViewingZenithAngle	G	D	
WavelengthRegistrationCheck	D		
WavelengthRegistrationCheckStd	D		
Weight			D
XTrackQualityFlags	D	D	

A Time calculations

The local mean, civil, or apparent time at the center of any OMI FOV can be obtained from the geolocation data, using the variable `Time` for the swath and the variable `Longitude` for the FOVÅpparent time requires, additionally, calculation of the Equation of Time. The `Time` variable is given in decimal TAI-93 format, so should be converted (for sub- minute precision) to UTC. The local solar times—mean and apparent—are of importance when the photochemical lifetimes of NO_2 are important. The relevant equations are:

$$\mathrm{UTC} = \mathrm{TAI} - 32 - \mathrm{LS} \quad (6)$$

$$\mathrm{LCT} = \mathrm{UTC} + \mathrm{TZ} \quad (7)$$

$$\mathrm{LMST} = \mathrm{UTC} + \lambda/15 \quad (8)$$

$$\mathrm{LAST} = \mathrm{LMST} + \mathrm{E} \quad (9)$$

Where

UTC	=	Coordinated Universal Time
LCT	=	Local civil time
LMST	=	Local mean solar time
LAST	=	Local apparent solar time
LS	=	Number of leap seconds added since July 1, 2004 One-second additions occurred at midnight after Dec. 31, 2005, Dec 31, 2008, Jun 30, 2012, Jun 30, 2015, and Dec 31, 2016)
TZ	=	Time zone value (*e.g.* −4 hours for U.S. Eastern Daylight Time)
λ	=	Longitude, in degrees (East positive, West negative)
E	=	Equation of Time

The Equation of Time, in minutes, can be approximated with a precision of < 6 s by the formula

$$\mathrm{E} = 9.87\sin(2B) - 7.53\cos(B) - 1.5\sin(B) \quad (10)$$

where

$$B = 360(\mathrm{DOY} - 81)/365 \quad (11)$$

$$\mathrm{DOY} = \text{Day of Year} \quad (12)$$

Formulae for higher-precision calculations of E can be found in various reference sources [Seidelmann, 2005].

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