

## OMBRO v3.0 File Specifications README

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This document lists all swath dimensions, geolocation fields, and data fields present in the SAO OMI data product files of the OMBRO PGE Algorithm Version v3.0 and higher (Collection/Product Version 003). **For OMBRO only**, it replaces OMSAO\_FileSpecifications\_README.odt, which holds for v2.0 of the PGE. The contents of this file are essentially a reformatted version of the File Specification (\*.fs files) documents which, together with more information on all PGEs, are available at <http://www.cfa.harvard.edu/atmosphere/SatelliteInstruments/OMI/PGEReleases/>.

Differing slightly from the format of OMSAO\_FileSpecifications\_README.odt, the last column of each table – formerly called “PGE” – now contains “Version” to indicate in which version (2.0 or 3.0) of the OMBRO product a data field is present.

### 1. Swath Dimensions

Name	Data Type	Dimension	Min. Value	Max Value	Description	Version
nTimes	I4	1	0	9999	Number of swath lines in the granule.	all
nXtrack	I4	1	0	60	Number of ground pixels per swath line.	all
nUTCdim	I4	1	6	6	Number of elements in a single <i>TimeUTC</i> field entry.	all

### 2. Geolocation Fields

Name	Data Type	Dimension	Min. Value	Max Value	Units	Description	Version
Latitude	R4	nXtrack,nTimes	-90.0	90.0	deg	The geodetic latitude at the center of the ground pixel.	all
Longitude	R4	nXtrack,nTimes	-180.0	180.0	deg	The geodetic longitude at the center of the ground pixel.	all
SolarAzimuthAngle	R4	nXtrack,nTimes	-180.0	+180.0	deg	The solar azimuth angle at the center of the ground pixel.	all
SolarZenithAngle	R4	nXtrack,nTimes	0.0	180.0	deg	The solar zenith angle at the center of the ground pixel.	all
SpacecraftAltitude	R4	nTimes	0.0e+00	1.0e+30	m	The altitude of the EOS-Aura satellite above WGS84 ellipsoid.	all
TerrainHeight	I2	nXtrack,nTimes	-1000	10000	m	The terrain height at the center of the ground pixel.	all
Time	R8	nTimes	0.0e+00	1.0e+10	s	The TAI93 time (in s) at the start of the swath line.	all
TimeUTC	I2	nUTCdim,nTimes	0	9999	n/a	UTC value of the TAI93 time at the start of the "scan". UTC time of format of the UTC string YYYY-MM-DD hh:mm:ss is divided into 6 integer fields containing  YYYY year (position 1) MM month (position 2) DD day (position 3) hh hours (position 4) mm minutes (position 5) ss seconds (position 6)	all
ViewingAzimuthAngle	R4	nXtrack,nTimes	-180.0	180.0	deg	The viewing azimuth angle ant the center of the ground pixel.	all
ViewingZenithAngle	R4	nXtrack,nTimes	0.0	180.0	deg	The viewing zenith angle ant the center of the ground pixel.	all
XtrackQualityFlags	I1	nXtrack,nTimes	0	127	n/a	Cross-track quality flags as set in L1b to flag the row anomaly.	3.0
XtrackQualityFlagsExpanded	I2	nXtrack,nTimes	0	11147	n/a	Human-readable version of <i>XtrackQualityFlags</i> .	3.0

### 3. Data Fields

Name	Data Type	Dimension	Min. Value	Max Value	Units	Description	Version
AMFCloudFraction	R4	nXtrack,nTimes	0.0	1.0	n/a	Cloud Fraction from the OMCLDO2 product, adjusted to fall within the range of [0,1]. Currently not used in OMBRO AMF computations.	3.0
AMFCloudPressure	R4	nXtrack,nTimes	0.0	1.0e+30	hPa	Cloud-Top pressure from the OMCLDO2 product. Currently NOT used in OMBRO AMF computations.	3.0
AdjustedSceneAlbedo	R4	nXtrack,nTimes	0.0	1.0	n/a	Average surface reflectance in OMI ground pixel. Used in OMBRO AMF look-up and computations.	3.0
AirMassFactor	R8	nXtrack,nTimes	0.0e+00	1.0e+30	n/a	Molecule specific air mass factor for each ground pixel; in the case of HCHO including scattering weights, clouds, and vertical distribution of HCHO. In the OMOCCLO product set to the geometric AMF.	all
AirMassFactorDiagnosticFlag	I2	nXtrack,nTimes	-2	13127	n/a	<p>Diagnostic flag for molecule specific air mass factor for each ground pixel. The flag indicates surface conditions and out of bound viewing geometry. Except for geometry and surface type, flag is computed additively, <i>i.e.</i>, it is the sum of all the conditions that apply to a ground pixel. Note that any of the cloud-related values below are applicable to OMHCHO only.</p> <p>Non-additive values</p> <ul style="list-style-type: none"> <li>= -2 Out of bounds viewing geometry, no AMF computation possible</li> <li>= -1 No table lookup possible; geometric AMF used instead</li> <li>= 0-100 NISE snow cover fraction</li> <li>= 101 NISE permanent ice</li> <li>= 103 NISE dry snow</li> <li>= 104 NISE ocean</li> <li>= 125 NISE suspect (no snow cover assumed)</li> <li>= 127 NISE error (no snow cover assumed)</li> </ul> <p>Additive values</p> <ul style="list-style-type: none"> <li>+ 1000 No OMI cloud fraction; use ISCCP climatology</li> <li>+ 2000 No OMI cloud top height; use ISCCP climatology</li> <li>+10000 Sun glint possibility; assume albedo of ice</li> </ul>	all
AirMassFactorGeometric	R8	nXtrack,nTimes	0.0e+00	1.0e+30	n/a	Geometric air mass factor for the viewing geometry of each ground pixel.	all
AverageColumnAmount	R8	1	-1.0e+30	1.0e+30	mol/cm <sup>2</sup>	Total column amount averaged over the the whole granule ("good" data only; see <i>MainDataQualityFlag</i> ).	all
AverageColumnUncertainty	R8	1	0.0e+00	1.0e+30	mol/cm <sup>2</sup>	Total column uncertainty averaged over the the whole granule ("good" data only; see <i>MainDataQualityFlag</i> ).	all
AverageFittingRMS	R8	1	0.0e+00	1.0e+30	n/a	Fitting RMS averaged over the the whole granule ("good" data only; see <i>MainDataQualityFlag</i> ).	all
ColumnAmount	R8	nXtrack,nTimes	-1.0e+30	1.0e+30	mol/cm <sup>2</sup>	Total column amount for each ground pixel.	all
ColumnAmountDestriped	R8	nXtrack,nTimes	-1.0e+30	1.0e+30	mol/cm <sup>2</sup>	Total column amount for each ground pixel after application of cross-track smoothing.	all
ColumnUncertainty	R8	nXtrack,nTimes	0.0e+00	1.0e+30	mol/cm <sup>2</sup>	Total column uncertainty for each ground pixel	all

Name	Data Type	Dimension	Min. Value	Max Value	Units	Description	Version
FitConvergenceFlag	I2	nXtrack,nTimes	-12	12344	n/a	<p>The flag indicating the type of (non-)convergence of the non-linear least squares fitting routine associated with the ground pixel.</p> <p>Exit integer scalar that indicates why the return is taken:</p> <ul style="list-style-type: none"> <li>=10000 convergence due to criterion no. 1 below</li> <li>= 2000 convergence due to criterion no. 2 below</li> <li>= 300 convergence due to criterion no. 3 below</li> <li>= 40 convergence due to criterion no. 4 below</li> <li>= x where x equals 0,1,2,3 or 4</li> <li>&lt; 0 indicates that no convergence criterion is fulfilled but some abnormal termination criterion is satisfied</li> <li>= -1 if <math>m &lt; n</math> or <math>n \leq 0</math> or <math>m \leq 0</math> or <math>mdc &lt; m</math> or <math>mdw &lt; n*n+5*n+3*m+6</math> or <math>maxit \leq 0</math> or <math>epsrel &lt; 0</math> or <math>epsabs &lt; 0</math> or <math>epsx &lt; 0</math> or invalid starting point on entry</li> <li>= -2 termination due to criterion no. 5</li> <li>= -3 termination due to criterion no. 6</li> <li>= -4 termination due to criterion no. 7</li> <li>= -5 termination due to criterion no. 8</li> <li>= -6 termination due to criterion no. 9</li> <li>= -7 there is only one feasible point, namely <math>x(i)=bl(i)=bu(i)</math> ; <math>i=1,2,\dots,n</math></li> <li>= -11 termination due to user stop indicator: fitting parameters out of bounds</li> <li>= -12 termination due to user stop indicator: "infinite loop" termination</li> </ul> <p>The convergence criteria are:</p> <ol style="list-style-type: none"> <li>1) relative predicted reduction in the objective function is less than <math>epsrel^{**2}</math></li> <li>2) the sum of squares is less than <math>epsabs^{**2}</math></li> <li>3) the relative change in x is less than <math>epsx</math></li> <li>4) we are computing at noise level the last digit in the convergence code (see below) indicates how the last steps were computed <ul style="list-style-type: none"> <li>= 0 no trouble (gauss-newton the last 3 steps)</li> <li>= 1 prank &lt; n at the termination point</li> <li>= 2 the method of newton was used (at least) in the last step</li> <li>= 3 the 2nd but last step was subspace minimization but the last two were gauss-newton steps</li> <li>= 4 the steplength was not unit in both the last two steps</li> </ul> </li> </ol> <p>The abnormal termination criteria are:</p> <ol style="list-style-type: none"> <li>5) no. of iterations has exceeded maximum allowed</li> </ol>	all

Name	Data Type	Dimension	Min. Value	Max Value	Units	Description	Version
						<p>iterations</p> <p>6) the hessian emanating from 2nd order method is not pos def</p> <p>7) the algorithm would like to use 2nd derivatives but is not allowed to do that</p> <p>8) an undamped step with newtons method is a failure</p> <p>9) the latest search direction computed using subspace minimization was not a descent direction (probably caused by wrongly computed Jacobian)</p> <p>Convergence constants and dimension parameters:</p> <p>maxit maximum number of allowed iterations</p> <p>tol pseudo rank tolerance constant</p> <p>epsrel relative convergence constant</p> <p>epsabs absolute convergence constant</p> <p>epsx parameter convergence constant</p> <p>n integer scalar containing the number of unknowns</p> <p>mdc integer scalar (mdc must be <math>\geq m</math>)</p> <p>m integer scalar containing the number of data points</p>	
FittingRMS	R8	nXtrack,nTimes	0.0e+00	1.0e+30	n/a	Fitting RMS for each ground pixel	all
MainDataQualityFlag	I2	nXtrack,nTimes	-1	2	n/a	<p>Main flag to indicate data quality. Its main purpose is to give the user of the data an easy way to screen for suspect or bad pixels. The possible values are:</p> <p><math>\leq -1</math> <i>Missing</i>: No columns have been computed; entries are missing.</p> <p>= 0 <i>Good</i>: Column values are present and pass all quality checks. Data may be used with confidence</p> <p>= 1 <i>Suspect</i>:: Data should be used with caution because one or more of the following quality checks failed:</p> <p>(a) <i>FitConvergenceFlag</i> is <math>&lt; 300</math> (but <math>\geq 0</math>)</p> <p>(b) Column+<math>2\sigma</math> uncertainty <math>&lt; 0.0</math> (but Column+<math>3\sigma</math> uncertainty <math>\geq 0.0</math>)</p> <p>(c) Absolute column value <math>&gt; \text{MaximumColumnAmount}</math></p> <p>= 2 <i>Bad</i>: Data should not be used, or used with extreme caution, because one or more of the following conditions are present:</p> <p>(a) <i>FitConvergenceFlag</i> is <math>&lt; 0</math> (abnormal termination of fitting)</p> <p>(b) Column+<math>3\sigma</math> uncertainty <math>&lt; 0.0</math></p>	all
MaximumColumnAmount	R8	1	0.0	1.0e+30	mol/cm <sup>2</sup>	Maximum absolute column amount up to which fitted columns qualify as "good" and beyond which they are considered	

Name	Data Type	Dimension	Min. Value	Max Value	Units	Description	Version
PixelArea	R4	nXtrack	0.0	4.133e+08	km <sup>2</sup>	"suspect" (see <i>MainDataQualityFlag</i> ). The area of tiled ground pixels. One representative value for each cross-track position is provided.	3.0
PixelCornerLatitudes	R4	nXtrack+1, nTimes+1	-90.0	90.0	deg	The geodetic latitudes of the corner coordinates of the OMI ground pixels.	all
PixelCornerLongitudes	R4	nXtrack+1, nTimes+1	-180.0	180.0	deg	The geodetic longitudes of the corner coordinates of the OMI ground pixels.	all
RadianceReferenceColumnAmount	R8	nXtrack	-1.0e+30	1.0e+30	mol/cm <sup>2</sup>	Slant column amount for each ground pixel in the reference swath line.	all
RadianceReferenceColumnUncertainty	R8	nXtrack	0.0e+00	1.0e+30	mol/cm <sup>2</sup>	Slant column amount uncertainty for each ground pixel in the reference swath line.	all
RadianceReferenceColumnXTRFit	R8	nXtrack	-1.0e+30	1.0e+30	mol/cm <sup>2</sup>	Cross-track fit to RadianceReferenceColumnAmount that is removed from the radiance reference spectrum in cases where the removal of the target gas from the reference spectrum has been selected.	all
RadianceReferenceConvergenceFlag	I4	nXtrack	-10	12344	n/a	The flag indicating the type of (non-) convergence of the non-linear least squares fitting routine for the radiance reference fit. See also <i>FitConvergenceFlag</i> .	all
RadianceReferenceFittingRMS	R8	nXtrack	0.0e+00	1.0e+30	n/a	Fitting RMS for each ground pixel in the radiance reference line.	all
RadianceReferenceLatitudeRange	R4	2	-90.0	+90.0	n/a	Lower and upper latitude values defining the range that went into the composition of the radiance reference spectrum. If equal, a single swath line was used with average latitude value closest to the specified latitudes.	all
RadianceWavCalConvergenceFlag	I2	nXtrack	-10	12344	n/a	The flag indicating the type of (non-) convergence of the non-linear least squares fitting routine for the radiance wavelength calibration. For a detailed description of the flag refer to <i>FitConvergenceFlag</i> .	all
RadianceWavCalLatitudeRange	R4	2	-90.0	90.0	n/a	Lower and upper latitude values defining the range that went into the composition of the radiance spectrum used for wavelength calibration. If equal, a single swath line was used with average latitude value closest to the specified latitudes.	all
SlantColumnAmount	R8	nXtrack,nTimes	-1.0e+00	1.0e+30	mol/cm <sup>2</sup>	Slant column amount for each ground pixel.	3.0
SlantColumnAmountDestriped	R8	nXtrack,nTimes	0.0e+00	1.0e+30	mol/cm <sup>2</sup>	Slant column amount for each ground pixel after application of a post-fitting destriping correction.	3.0
SlantColumnUncertainty	R8	nXtrack,nTimes	0.0e+00	1.0e+30	mol/cm <sup>2</sup>	Slant column amount uncertainty for each ground pixel.	3.0
SlantFitConvergenceFlag	I2	nXtrack,nTimes	-12	12344	n/a	The flag indicating the type of (non-) convergence of the non-linear least squares fitting routine for the slant column fit. For a detailed description of the flag refer to <i>FitConvergenceFlag</i> .	3.0
SlantFittingRMS	R8	nXtrack,nTimes	0.0e+00	1.0e+30	n/a	Slant Fitting RMS for each ground pixel.	3.0
SolarWavCalConvergenceFlag	I2	nXtrack	-12	12344	n/a	The flag indicating the type of (non-) convergence of the non-linear least squares fitting routine for the solar wavelength calibration. For a detailed description of the flag refer to <i>FitConvergenceFlag</i> .	all

#### 4. Global Metadata

Name	Data Type	Dimension	Min. Value	Max Value	Units	Description/Value	Version
AuthorAffiliation	Char	1	n/a	n/a	n/a	"Smithsonian Astrophysical Observatory"	all
AuthorName	Char	1				"Thomas P. Kurosu"	all
GranuleDay	I4	1	1	31	n/a	The day of the month at the start of the granule.	all
GranuleMonth	I4	1	1	12	n/a	The month at the start of the granule.	all
GranuleYear	I4	1	2003	2099	n/a	The (four-digit) year at the start of the granule.	all
HDFEOSVersion	Char	1	n/a	n/a	n/a	Example is "HDFEOS 5.1.12".	all
InputVersions	Char	1	n/a	n/a	n/a	A list of every ESDT (including version) whose product was used as input for the processing.	all
InstrumentName	Char	1	n/a	n/a	n/a	"OMI"	all
FittingWindowLimits	R4	6	0.0	500.0	nm	1: First wavelength of total wavelength interval 2: First wavelength of fitting window considered in fit 3: Last wavelength of fitting window considered in fit 4: Last wavelength of total wavelength interval 5: First wavelength of any interval excluded from fit 6: Last wavelength of any interval excluded from fit Numbers 2 and 3 define the actual fitting window, bracketed by numbers 1 and 4 (usually +/-2nm on each end). Numbers 5 and 6 are ignored if there is no overlap with the fitting window.	all
NumberOfBadOutputSamples	I4	1	0	2147483647	n/a	Number of measurement pixels in granule for which retrieval was performed and quality status is 'bad'.	all
NumberOfConvergedSamples	I4	1	0	2147483647	n/a	Number of measurement pixels in granule for which the non-linear least squares fit converged.	all
NumberOfExceededIterationsSamples	I4	1	0	2147483647	n/a	Number of measurement pixels in granule for which the non-linear least squares fit failed to converge because the maximum number of allowed iterations was exceeded.	all
NumberOfFailedConvergenceSamples	I4	1	0	2147483647	n/a	Number of measurement pixels in granule for which the non-linear least squares fit failed to converge.	all
NumberOfGoodOutputSamples	I4	1	0	2147483647	n/a	Number of measurement pixels in granule for which retrieval was performed and quality status is 'good'.	all
NumberOfInputSamples	I4	1	0	2147483647	n/a	Number of measurement pixels in granule on which retrieval is performed.	all
NumberOfOutOfBoundsSamples	I4	1	0	2147483647	n/a	Number of measurement pixels in granule for which the retrieved columns are "out of bounds", i.e., negative within 3 $\sigma$ retrieval uncertainties.	all
NumberOfScanLines	I4	1	0	2147483647	n/a	Number of scan lines in radiance granule.	all
NumberOfSuspectOutputSamples	I4	1	0	2147483647	n/a	Number of measurement pixels in granule for which retrieval was performed and quality status is 'suspect'.	all
OrbitData	Char	1	n/a	n/a	n/a	Indicates whether orbit data used by the L1B processor is definitive or predicted.	all
PercentBadOutputSamples	R4	1	0.0	100.0	n/a	Percentage of performed retrievals with quality status 'bad'.	all
PercentGoodOutputSamples	R4	1	0.0	100.0	n/a	Percentage of performed retrievals with quality status 'good'.	all
PercentSuspectOutputSamples	R4	1	0.0	100.0	n/a	Percentage of performed retrievals with quality status 'suspect'.	all
PGEVERSION	Char	1	n/a	n/a	n/a	Actual is "3.0.2".	all
ProcessingCenter	Char	1	n/a	n/a	n/a	Example is "OMIDAPS".	all
ProcessLevel	Char	1	n/a	n/a	n/a	Actual is "2".	all
SpaceCraftMaxAltitude	R8	1	0.0e+00	1.0e+30	m	Maximum elevation of the Aura space craft.	all
TAI93At0zOfGranule	R8	1	0.0e+00	1.0e+30	s	The TAI93 time at 0z of the granule.	all

## 5. Swath Metadata

Name	Data Type	Dimension	Min. Value	Max Value	Units	Description	Version
EarthSunDistance	R8	1	1.47e+11	1.53e+11	m	The Earth-sun distance at the time of the irradiance measurement.	all
SwathName	Char	1	n/a	n/a	n/a	"OMI Total Column Amount BrO"	all
VerticalCoordinate	Char	1	n/a	n/a	n/a	"Total Column"	all