TITLE:

# Ozone_cci+

# Product User Guide
# (PUG v2.1)

**Date of issue:** 17/03/2025
**Version**: 2.1
**Reference**: Ozone_cci+_D4.2_PUG_v2.1
**Distributed to**: Ozone_cci+ Consortium

**WP Manager:** A. Keppens
**WP Manager Organization**: BIRA-IASB
**Other partners:** DLR-IMF, KNMI, RAL, ULB, IUP-UB, FMI

## DOCUMENT PROPERTIES

| | |
|---|---|
| **Title** | Ozone_cci+ Product User Guide (PUG) |
| **Reference** | Ozone_cci+_D4.2_PUG_v2.1 |
| **Issue** | 2 |
| **Revision** | 1 |
| **Status** | Final |
| **Date of issue** | 17/03/2025 |
| **Deliverable** | D4.2 |

| | FUNCTION | NAME | DATE | SIGNATURE |
|---|---|---|---|---|
| LEAD AUTHORS | Scientists | Carlo Arosio<br>Viktoria Sofieva<br>Melanie Coldewey-Egbers<br>Klaus-Peter Heue<br>Catherine Wespes<br>Ronald van der A<br>Richard Siddans | 04/11/2024 | |
| EDITOR | | Catherine Wespes<br>Rosa Astoreca | 04/11/2024 | |
| APPROVED BY | ESA | Michael Eisinger | 05/03/2025 | |
| ISSUED BY | Science Leader | Daan Hubert | 17/03/2025 | |

## DOCUMENT CHANGE RECORD

| Issue | Revision | Date | Modified items | Observations |
|---|---|---|---|---|
| 01 | 00 | 19/10/2021 | | |
| 01 | 01 | 24/06/2022 | | |
| 02 | 00 | 06/11/2024 | All sections | |
| 02 | 01 | 17/03/2024 | Document header | Approved by ESA |

# Table of Contents

# 1. Purpose and scope

The Product User Guideline (PUG) is a deliverable of the ESA Ozone_cci+ project (https://climate.esa.int/en/projects/ozone). The Ozone_cci+ project aims to deliver Essential Climate Variable (ECV) Ozone products in line with the "Systematic observation requirements for satellite-based products for climate" as defined by GCOS (Global Climate Observing System) in (GCOS-107 2006): "Product A.7: Profile and total column of ozone".

The purpose of this document is to describe the ozone products generated in the framework of Ozone_cci+ Phase 2 (2022-2024), including a detailed description of the file format and their use.

# 2. Overview of Ozone_cci+ Phase 2 products

The Ozone_cci+ Phase 2 includes data products for total ozone columns, tropospheric ozone columns as well as ozone profiles from nadir sensors and from from limb and occultation sensors (Table 2.1). All data sets are provided in netCDF-4 CF format following CCI data standards and are freely available on the Ozone_cci website (https://climate.esa.int/en/projects/ozone/data).

**Table 2.1: List of the Ozone_cci+ Phase 2 datasets and associated characteristics**

| Product identifier | Source/ Processing center | Time period | Altitude range | Spatial resolution | Temporal resolution | Uncertainty |
|---|---|---|---|---|---|---|
| **Level-2 Data Sets** | | | | | | |
| NP_L2_IASIA_CDR<br>Sects 3.5 & 4.5 | EUMETSAT | 2008-2019 | 0-60 km | IASI pixel (4 observations with a footprint of 12 km every 50 km).<br>N.B.: 3 to 4 pixels /10 are processed for now | Bi-daily (morning and afternoon overpass times) | Variable with latitude and season (usually <15% in the stratosphere and ~10-35% in the troposphere) |
| NP_L2_IASIB_CDR<br>Sects 3.5 & 4.5 | EUMETSAT | 2020-2023 | 0-60 km | IASI pixel (4 observations with a footprint of 12 km every 50 km).<br>N.B.: 3 to 4 pixels /10 are processed for now | Bi-daily (morning and afternoon overpass times) | Variable with latitude and season (usually <15% in the stratosphere and ~10-35% in the troposphere) |
| LP_L2_OMPS_N21<br>Sects 3.8 and 4.8 | IUP-UB | 2023/02 - 2023/12 | 8.5 - 60.5 km | ~1° latitude, switch to ~0.5° from Dec 12 | 15 s (day side of the orbit only) 8 s from Dec 12 | Retrieval noise within ±5% between 20 and 60 km |
| **Level-3 Data Sets** | | | | | | |

| Product identifier | Source/ Processing center | Time period | Altitude range | Spatial resolution | Temporal resolution | Uncertainty |
|---|---|---|---|---|---|---|
| TTOC_L3_GTTO_MRG<br>Sects 3.2 and 4.2 | DLR | 1995/07 - 2023/12 | Surface to 270 hPa or 200 hpa | 1° x 1° | Monthly | ~1.5 mmol/m² |
| LNTOC_L3_GTO<br>Sects 3.3 and 4.3 | FMI | 2002-2023 | Surface to LRT or LRT-3 km | 1° x 1° | Monthly | tbd |
| LNTOC_L3_OMI<br>Sects 3.3 and 4.3 | FMI | 2004-2023 | Surface to LRT or LRT-3 km | 1° x 1° | Monthly | tbd |
| NP_L3_GOP_MRG<br>Sects 3.4 and 4.4 | DLR | 07/1995-10/2021 | 0-80 km | 5° x 5° | Monthly | tbd |
| NP_L3_IASI_MRG<br>Sects 3.6 and 4.6 | ULB | 2008-2023 | 0-60 km | 1° x 1° | Daily | Variable with altitude, latitude, season; it reflects the number of original measurements merged in the 1°x1° bin and associated retrieval uncertainties. Usually <5% in the stratosphere and <15% in the troposphere |
| LP_L3_HIRES<br>Sects 3.7 and 4.7 | FMI | 2002-2023 | 900-0.02 hPa | 1° x 1° | Daily | tbd |
| **Level-4 Data Sets** | | | | | | |
| TC_L4_MSR<br>Sects 3.1 and 4.1 | KNMI | 1960-2023 | Total column | 0.5 ° x 0.5 ° | Monthly | Variable |

# 3. Data processing and parameters

This section describes the details of the total ozone, tropospheric ozone, nadir profile and limb profile ECV datasets, including the attributes of the data and algorithms used. For a full technical description of the retrieval algorithm used please consult the Ozone_cci+ Algorithm Theoretical Basis Document (ATBD, https://climate.esa.int/en/projects/ozone/key-documents).

## *3.1. Multi-Sensor Reanalysis 2 (Level-4) (KNMI)*

### 3.1.1. Input data and algorithm

A single coherent total ozone data set (the Ozone-MSR version 2; van der A et al., 2015) has been created from all available ozone column data measured by polar orbiting satellites in the near-ultraviolet Huggins band in the last four decades. In total 19 satellite data sets were used in the assimilation run, including BUV-Nimbus4, TOMS-Nimbus7, TOMS-EP, SBUV-7, -9, -11, -14, -16, -17, -18, -19, GOME, SCIAMACHY, OMI, GOME-2A, GOME-2B, GOME-2C, OMPS and TROPOMI. For the years 1957-1970 data from the Dobson stations is used as input.

The ozone MSR is produced in two steps. First, the latest reprocessed versions of all available ozone column satellite datasets are collected, and are corrected for biases as function of solar zenith angle, viewing angle, time (trend), and stratospheric temperature using Brewer/Dobson ground measurements from the World Ozone and Ultraviolet Radiation Data Centre (WOUDC). The list of stations can be found in van der A et al. (2015). Subsequently the debiased satellite observations are assimilated within the ozone chemistry and data assimilation model TMDAM driven by meteorological analyses of the European Centre for Medium-Range Weather Forecasts (ECMWF).

### 3.1.2. Parameters

In Tables 3.1.1 and 3.1.2 (metadata and data), the content of the data file is explained.

**Table 3.1.1: Meta data of the MSR netCDF file.**

| Parameter | Description |
|---|---|
| CDI | Climate Data Interface version |
| Conventions | Convention versions |
| History | Input of individual monthly mean data files |
| Authors | Person(s) responsible for the MSR data processing |
| Email | Email address of the contact person |
| Data_created_by | Software version |
| Ozone_field_date | Start date of the data set |
| Date_format | Format of the date |
| Number_of_longitudes | Number of grid cells in longitude direction |
| Longitude_range | Range of longitude values |
| Longitude_step | Resolution of the data in longitude direction |
| Number_of_latitudes | Number of grid cells in latitude direction |
| Latitude_range | Range of latitude values |
| Latitude_step | Resolution of the data in latitude direction |
| Field_Average_O3_column | Description of the ozone data |

| Parameter | Description |
|---|---|
| Field_Average_O3_std | Description of the ozone uncertainty data |
| Units | Unit of the ozone data |
| Undefined_value | Flag value of undefined data points |
| Datefile_generated_at | Production date of the data |
| Note | Additional information |
| CDO | Version of the Climate Data Operators |

**Table 3.1.2: Variables of the MSR netCDF file. $N_{date}$, $N_{lat}$, $N_{lon}$ are number of months, latitudes and longitudes, respectively.**

| Parameter | Unit | Dimension | Description |
|---|---|---|---|
| Time | Month | $N_{date}$ | months since January 1960 |
| Latitude | degrees north | $N_{lat}$ | Center latitude of grid cell |
| Longitude | degrees east | $N_{lon}$ | Center longitude of grid cell |
| Monthly average of ozone column | DU | $N_{date} \times N_{alt} \times N_{lat}$ | Total column per grid cell |
| Standard deviation of monthly average ozone column | DU | $N_{date} \times N_{alt} \times N_{lat}$ | Uncertainty of the total column |

## 3.2. *Tropical Tropospheric Ozone CCD (Level-3) (DLR)*

### 3.2.1. Input data and algorithm

The GODFIT Total ozone columns from the sensors GOME, SCIAMACHY, GOME-2 (A, B, C), OMI and S5P are used as input for a convective cloud differential algorithm together with the respective cloud data. The total column product and retrieval are described in PUG v1.1 (https://climate.esa.int/documents/1729/Ozone_cci_D4.2_PUG_V1.1.pdf).

The CCD algorithm was applied to the total ozone columns in the second phase of Ozone CCI as described in Heue et al. (2016). The stratospheric ozone column is estimated by the ozone column above deep convective clouds. As the cloud top pressure varies, we add an ozone climatology column between the cloud height and a fixed top level. We offer two different versions of the dataset with 200 and 270 hPa to be comparable with the old version as well as with the operational S5P data product.

Most deep convective clouds are observed between the Gulf of Bengal and New Guinea (70°E to 170°W), so we use this region as reference to calculate the stratospheric column, the assumption that the same stratospheric column can be used for a certain latitude band limits the algorithm to the tropical band (20°S to 20°N). The difference between the total column for cloud free observations and the stratospheric column results in the tropospheric residual. The tropospheric columns are gridded to 1°x 1° resolution. The propagated error from the total and stratospheric columns as well as the standard deviation of all tropospheric columns in a grid cell are given as error and uncertainty, respectively. Dividing the tropospheric column by the pressure difference between the top level and the surface pressure, and some constant factors, results in a mean tropospheric mixing ratio.

The data are harmonized to OMI as reference instrument by adding the tropical mean annual difference between the individual sensors and OMI. GOME data in the complete tropical belt are available only until June 2003, therefore, they do not overlap with OMI and we use the harmonized SCIAMACHY data as reference for GOME. The mean tropospheric column of harmonized data is given as final result. Once the tropospheric column is harmonized, the mixing ratio is multiplied with the tropical mean ratio between harmonized columns and original data for each sensor. Again, the mean of the harmonized mixing ratio is given as final result.

For both columns and mixing ratios, the errors are propagated from the errors of the individual monthly CCD data by the root mean square. The error is therefore based on the propagated error from the total and the stratospheric columns.

For each sensor a qa-value is retrieved based on the number of observations per ground pixel. By default the qa is set to unity but is reduced by 12.5% if the data in the stratospheric reference are flagged for each flag, the respective thresholds are given in the METADATA/ ALGORITHM_SETTINGS. The minimum value if all stratospheric flags were set reaches 0.5, by definition this will affect the complete latitude band. The quality value of individual ground pixels is further reduced if thresholds are not met for the error of the data point, the number of negative tropospheric residual or total number, as shown in the following table.

**Table 3.2.1: Threshold and qa reduction of individual ground pixels.**

| | **Threshold** | **qa reduction** |
|---|---|---|
| Error of pixel | 6e-3 | 0.15*(error/threshold) |
| Number of total pixels | 5 | 0.10*(threshold/#total) |
| Negative data | -- | 0.25*(#neg/#total) |

For S5P the operational CCD data product is used and averaged to the 1° x 1° x 1 month resolution or in case of the 200 hPa product a similar intermediate product is retrieved with the same algorithm except that the top level is set to 200 hPa. For the definition of the respective qa-values the PUG of the operational product is recommended (available at: https://sentiwiki.copernicus.eu/web/s5p-products).

During the harmonisation only data with qa values higher than 70% are considered for all instruments. The final qa value is the mean of the qa higher than 70% and is therefore by definition higher than 70%. If no sensor has data for a respective grid cell, the qa is set to zero.

### 3.2.2. Parameters

The main PRODUCTS in the merged data file are given below.

**Table 3.2.2: List of variables in the merged data file**

| | **Unit** | **Datatype** | **Reasonable range** |
|---|---|---|---|
| tropospheric_ozone_column | $mol/m^2$ | float | 0-30 e-3 |
| tropospheric_ozone_column_error | $mol/m^2$ | float | 0 – 10 e-3 |
| tropospheric_ozone_column_number | 1 | int | 0 -10000 |
| tropospheric_ozone_mixingratio | nmol/mol (ppb) | float | 0 - 100 |
| tropospheric_ozone_mixingratio_error | nmol/mol (ppb) | float | 0 - 30 |
| qa_value | 1 | float | 0-1 |

In addition, the SUPPORT_DATA DETAILED_RESULTS for the individual sensors are listed before the harmonisation:

**Table 3.2.3: SUPPORT_DATA DETAILED_RESULTS for the individual sensors**

| | **Unit** | **Datatype** | **Reasonable range** |
|---|---|---|---|
| tropospheric_ozone_column sensors | $mol/m^2$ | float | 0-30 e-3 |
| tropospheric_ozone_column_error sensors | $mol/m^2$ | float | 0 – 10 e-3 |
| tropospheric_ozone_column harmonisation sensors | $mol/m^2$ | float | ± 2 e-3 |
| tropospheric_ozone_mixingratio sensors | nmol/mol (ppb) | float | 0 - 80 |
| tropospheric_ozone_mixingratio_error senors | nmol/mol (ppb) | float | 0 - 30 |
| qa_value sensors | 1 | float | 0-1 |

The tropospheric columns in this group are stored as non harmonized data, to retrieve the harmonized data for each sensor, the tropospheric_ozone_column harmonization sensors has to be added to the tropospheric_ozone_column sensors variable (see Section **Error! Reference source not found.**).

Moreover, additional data like SURFACE_PROPERTIES (land water mask and albedo) or the STRATOSPHERIC OZONE (harmonized reference columns) and the TOTAL_OZONE (sum of harmonized tropospheric and harmonized stratospheric column) are given.

## *3.3. Limb-Nadir matched Tropospheric Ozone (Level-3) (FMI)*

### 3.3.1. Input data and algorithm

The tropospheric ozone column from a combination of nadir and limb instruments is obtained via the residual method, i.e., the stratospheric ozone column is subtracted from the total ozone column.

OMI or GTO are used for total ozone column data. The stratospheric ozone column is computed either from the tropopause or from 3 km below the tropopause using the high-resolution gap-free dataset of ozone profiles LIMB-HIRES.

Once the high-resolution stratospheric ozone column dataset is created, the application of the residual method is straightforward: the stratospheric columns are subtracted from the clear-sky measurements by the nadir sensors, daily. The daily values can be averaged to monthly mean values subsequently.

### 3.3.2. Parameters

The OMI-LIMB and GTO-LIMB tropospheric ozone column data are monthly means collected in the corresponding monthly netCDF files. For example, the file ESACCI-OZONE-LP-TrOC_LNM-GTO_LIMB_v1_200410_fv001.nc contains GTO-LIMB data for October 2004.

The structure of this file is below. The structure of the OMI-LIMB files is similar.

**Table 3.3.1: List of variables in the OMI-LIMB netCDF files**

| **Parameter** | **Unit** | **Dimension** | **Description** |
|---|---|---|---|
| latitude | degrees north | $N_{lat} \times 1$ | centers of latitude bins |
| longitude | degrees east | $N_{lon} \times 1$ | centers of longitude bins |
| TrOC_belowTP | DU | $N_{lat} \times N_{lon}$ | tropospheric ozone column from ground to 3 km below the tropopause |
| TrOC_belowTP_error | DU | $N_{lat} \times N_{lon}$ | estimated random error of tropospheric ozone column from ground to 3 km below tropopause |

| Parameter | Unit | Dimension | Description |
|---|---|---|---|
| | | | |
| TrOC_TP | DU | $N_{lat} \times N_{lon}$ | tropospheric ozone column from ground to the tropopause |
| TrOC_TP_error | DU | $N_{lat} \times N_{lon}$ | estimated random error of tropospheric ozone column from ground to the tropopause |
| number_of_data | 1 | $N_{lat} \times N_{lon}$ | number of data in lat-lon bins for this month |
| tropopause_height | km | $N_{lat} \times N_{lon}$ | mean tropopause height in the considered month computed using ERA-5 temperature |
| tropopause_pressure | hPa | $N_{lat} \times N_{lon}$ | mean tropopause pressure in the considered month computed using ERA-5 pressure |

## *3.4. UV-visible Merged Ozone Profile (Level-3) (DLR)*

### 3.4.1. Input data and algorithm

Data from the uv-visible nadir sensors listed in the table below are merged into a single cohesive record GOP-ECV. Before the merging, adjustments are applied to the individual sensors in order to correct for inter-sensor biases and drifts. OMI is used as a reference sensor. In a final step the merged profiles are scaled using as a reference the total column from the GTO-ECV product (Coldewey-Egbers et al., 2015).

**Table 3.5.1: List of input data used for the generation of the merged GOP-ECV record. Note that time coverage corresponds to the period for which the data is included in GOP-ECV.**

| Sensor | Time coverage | Level-3 data | RAL Level-2 Algorithm |
|---|---|---|---|
| GOME/ERS-2 | 07/1995 – 12/2002 | fv0006 | fv0301 |
| SCIAMACHY/ENVISAT | 08/2002 – 12/2004 | fv0006 | fv0300 |
| GOME-2/METOP-A | 01/2007 – 12/2016 | fv0006 | fv0300 |
| GOME-2/METOP-B | 01/2015 – 10/2021 | fv0007/fv0008 | fv0303/fv0305 |
| OMI/AURA | 10/2004 – 10/2021 | fv0006/fv0007 | fv0214 |

### 3.4.2. Parameters

GOP-ECV merged profile data are stored in netCDF files.

**Table 3.5.2: List of variables in the GOP-ECV netCDF files**

| Parameter | Unit | Dimension | Description |
|---|---|---|---|
| time | days | $N_{time} \times 1$ | Days since start of month |
| latitude | degrees north | $N_{lat} \times 1$ | Latitude of grid cell center |
| longitude | degrees east | $N_{lon} \times 1$ | Longitude of grid cell center |
| pressure | hPa | $N_{level} \times 1$ | Pressure levels of retrieved ozone profiles |
| ozone_total_column | DU | $N_{time} \times N_{lat} \times N_{lon}$ | Ozone total column |
| ozone_partial_column | DU | $N_{time} \times N_{layer} \times N_{lat} \times N_{lon}$ | Ozone partial column |
| ozone_partial_column _uncertainty | DU | $N_{time} \times N_{layer} \times N_{lat} \times N_{lon}$ | Ozone partial column uncertainty |

## *3.5. IASI Ozone Profile CDR (Level-2) (ULB)*

### 3.5.1. Input data and algorithm

The IASI instrument is a Fourier transform spectrometer that measures the thermal infrared emission of the Earth-atmosphere system between 645 and 2760 $cm^{-1}$ with a spectral resolution of 0.5 $cm^{-1}$. IASI provides global coverage of the Earth twice a day (at 9:30 and 21:30 mean local solar time) with a set of four simultaneous footprints of 12 km diameter at nadir.

The IASI L2 $O_3$ CDR product has been generated at EUMETSAT using the FORLI-$O_3$ (Fast Optimal Retrieval on Layers for IASI; v20151001) retrieval algorithm (Hurtmans et al., 2012). FORLI relies on a fast radiative transfer and retrieval methodology based on the Optimal Estimation Method (Rodgers, 2000). FORLI operates with multiplication factors, with the *a priori* as reference, and the profile is adjusted in layer partial columns. The IASI L2 $O_3$ CDR product is a profile retrieved on 40 layers between the surface and 40 km, with an extra layer from 40 to 60 km, the top of the atmosphere (TOA). It is provided along with associated averaging kernels and retrieved total errors on the same vertical grid.

The IASI L2 $O_3$ CDR dataset is, for now, processed at EUMETSAT for the period 2008 - 2023 running FORLI-$O_3$ (v20151001) on daily L1C radiances from two of the three IASI instruments: IASI/Metop-A from 2008 to 2019 (reprocessed L1C until December 2016 - doi = 10.15770/EUM_SEC_CLM_0014 – and operational L1C, which has no doi, onwards) and IASI/Metop-B (operational L1C; no doi) from 2020 to 2023, with the IASI L2 data that were reprocessed by EUMETSAT (with an adapted version of the EUMETSAT operational algorithm V6.6) to produce an homogeneous CDR (Release 1 IASI L2), used as inputs in FORLI-$O_3$.

The IASI L2 $O_3$ CDR is produced for twice daily measurements, but only 3 to 4 pixels over 10, due to computing constraints.

The reader is invited to refer to documentation available at https://climate.esa.int/en/projects/ozone/key-documents (ATBD) and to Hurtmans et al. (2012) for a full description of the retrieval parameters/input data and of the performances of the retrieval algorithm.

The FORLI-$O_3$ software v20151001 (Hurtmans et al., 2012) was implemented at EUMETSAT in 2019 and the current IASI L2 $O_3$ CDR product (as described above) has been recently distributed via EUMETCast (in netCDF format) using principal component compression (PCC). The EUMETSAT IASI L2 $O_3$ CDR files are then reformatted by LATMOS in netCDF format after data reconstruction and should be distributed by AERIS (https://iasi.aeris-data.fr/O3) in a near future. The last FORLI-$O_3$ release (v20191122) is not implemented yet at EUMETSAT.

### 3.5.2. Parameters

Table 3.6.1 describes the variables contained in the IASI L2 $O_3$ CDR output netCDF files (available from 2008 to 2023) that are reformatted by LATMOS.

**Table 3.6.1: Variables in the IASI L2 O3 CDR netCDF files reformatted by LATMOS. Time denotes number of IASI observations, nlayers denotes the number of retrieved vertical layers and npressures the number of pressure levels used to define inversion layers**

| Variable | Unit | Dimensions | Description / Comment |
|---|---|---|---|
| Time | day | time | UTC observation time in days since 1970-01-01 00:00:00 UTC |
| AERIStime | second | time | UTC observation time in seconds since 2007-01-01 00:00:00 UTC |
| Hour | hour | time | UTC observation hour of the day |
| Minute | minute | time | UTC observation minute of the hour |
| Second | second | time | UTC observation second of the minute |
| Latitude | degree_north | time | Latitude of ground pixel center |
| Longitude | degree_east | time | Longitude of ground pixel center |
| solar_zenith_angle | degree | time | solar zenith angle at the Earth's surface for the pixel center |
| satellite_zenith_angle | degree | time | Metop zenith angle at the Earth's surface for the pixel center |
| orbit_number | | time | Metop orbit number |
| scanline_number | | time | Scanline number in the Metop orbit |
| pixel_number | | time | Pixel number in the current scanline |
| ifov_number | | time | Field of view number in the 2 x 2 observation matrix |
| retrieval_quality_flag | | time | Retrieval quality flag summarizing processing flags. 2 for the most reliable pixels, not used for the moment; = 1 for the valuable pixels; = 0 for the remaining pixels that we recommend not to use |
| surface_altitude | m | time | Altitude of the surface |
| tropopause_altitude | m | time | Altitude of the tropopause |
| O3_apriori_partial_column _profile | mol $m^{-2}$ | time x nlayers | Ozone a priori partial column vertical profile in mole/m2 in the layers defined by the levels given in the variable atmosphere_pressure_grid |
| O3_partial_column_profile | mol $m^{-2}$ | time x nlayers | Ozone partial column vertical profile in mole/m2 retrieved in the layers defined by the levels given in the variable atmosphere_pressure_grid |
| O3_partial_column_profile _error | | time x nlayers | vertical profile of total retrieval error associated to ozone partial column vertical profile in the layers defined by the levels given in the variable atmosphere_pressure_grid |
| O3_total_degrees_of _freedom | | time | Degrees of freedom of the signal in the retrieved ozone partial column profile |
| air_partial_column_profile | mol $m^{-2}$ | time x nlayers | Air partial column vertical profile in mole/m2 in the layers defined by the levels given in the variable atmosphere_pressure_grid |

| Variable | Unit | Dimensions | Description / Comment |
|---|---|---|---|
| atmosphere_pressure_grid | Pascal | time x npressures | Pressures in Pa corresponding to levels used to define inversion layers: 40 layers of about 1 km height between Earth' s surface and 40 km with an additional layer from 40 km to the top of the atmosphere (60 km) |
| averaging_kernel_matrix | | time x nlayers x Nlayers | Ozone partial column averaging kernels matrix ((mol/m2)/(mol/m2)) in the layers defined by the levels given in the variable atmosphere_pressure_grid. |

## *3.6. IASI Merged Ozone Profile (Level-3) (ULB)*

### 3.6.1. Input data and algorithm

The L3 IASI merged ozone profile dataset is created using the daily L2 IASI/Metop-A, -B and -C $O_3$ profile dataset generated at ULB using the latest version of the original FORLI-O3 (v20191122) retrieval datasets (Hurtmans et al., 2012).

The L3 IASI merged $O_3$ dataset is processed at ULB-LATMOS for the period 2008 - 2023 running on FORLI-O3 profiles from IASI/Metop-A over 20080101-20190919, from IASI/Metop-B over 20130308-20231231 and from IASI/Metop-C over 20190920-20231231. It consists of daily partial columns profiles in 1° latitude x 1°longitude bins from 90°S to 90°N and from 180°W to 180°N, and from the surface to the top of atmosphere in 40 layers of about 1 km height between the surface and 40 km with one extra layer from 40 to 60 km.

The L3 IASI merged $O_3$ profile is created by weighted averaging of the FORLI-O3 profiles from individual IASI instruments assigned to the 1°x1° bins and for each layers. The weights used for the averaging are the reciprocal square of the total retrieval errors associated to the retrieved partial columns profile. The details of computing merged partial columns profiles from individual instruments with associated uncertainty can be found in the End to End ECV Uncertainty Budget document (E3UB v6.0, https://climate.esa.int/en/projects/ozone/key-documents).

The L3 IASI merged $O_3$ files are provided by ULB in netCDF format and distributed by ULB and LATMOS.

### 3.6.2. Parameters

The variables contained in the L3 IASI merged O3 output netCDF files (available from 2008 to 2023) are collected in Table 3.7.1.

**Table 3.7.1: Variables in the L3 IASI merged O3 netCDF files produced by ULB. Nlon, Nlat, Npressure and Nayers denote number of IASI observations, nlayers denotes the number of longitude and latitude zones, of pressure levels used to define inversion layers and of retrieved vertical layers.**

| Variable | Unit | Dimensions | Description / comment |
|---|---|---|---|
| longitude | degrees_east | Nlon | Centers of longitude bins: -179.5°:1°:179.5° |
| latitude | degrees_north | Nlat | Centers of latitude bins: -89.5°: 1°:89.5° |

| Variable | Unit | Dimensions | Description / comment |
|---|---|---|---|
| surface_altitude | km | Nlat x Nlon | Mean surface altitude in 1°x1° bin |
| atmosphere_pressure_grid | Pascal | Nlat x Nlon x Npressures | Mean pressures in Pa in the 1°x1° bin corresponding to levels used to define the inversion layers: 40 layers of about 1 km height between Earth's surface and 40 km, with one extra layer from 40 to the top of the atmosphere (60 km). |
| O3_total_column | mol $m^{-2}$ | Nlat x Nlon | Merged integrated total O3 columns in mole/$m^2$ calculated as the weighted average of all values assigned to the 1°x1° bin; The weights used for the averaging are the reciprocal square of the total retrieval errors associated with the retrieved total columns. |
| O3_total_column_error | mol $m^{-2}$ | Nlat x Nlon | Uncertainty in mole/$m^2$ associated with the weighted average of integrated total O3 columns in the 1°x1° bin, calculated as the reciprocal square root of the sum of all the individual weights, with the reciprocal square of the total retrieval errors associated with the retrieved total columns as weights. |
| O3_partial_column_profile | mol $m^{-2}$ | Nlat x Nlon x Nlayers | Merged ozone partial column vertical profile in mole/$m^2$ retrieved in the layers defined by the levels given in the variable atmosphere_pressure_grid and calculated as the weighted average of all values assigned to the 1°x1° bin and for each layer; The weights used for the averaging are the reciprocal square of the total retrieval errors associated with the partial columns retrieved in each layer. |
| O3_partial_column_error_profile | mol $m^{-2}$ | Nlat x Nlon x Nlayers | Uncertainty in mole/$m^2$ associated with the weighted average of O3 partial column vertical profile in the 1°x1° bin and for each layer, calculated as the reciprocal square root of the sum of all the individual weights, with the reciprocal square of the total retrieval errors associated with the partial columns retrieved in each layer as weights. |
| O3_apriori_partial_column_profile | mol $m^{-2}$ | Nlat x Nlon x Nlayers | O3 a priori partial column vertical profile in mole/$m^2$ in the layers defined by the levels given in the variable atmosphere_pressure_grid. |
| air_partial_column_profile | mol $m^{-2}$ | Nlat x Nlon x Nlayers | Merged air partial column vertical profile in mole/$m^2$ in the layers defined by the levels given in the variable atmosphere_pressure_grid |

| Variable | Unit | Dimensions | Description / comment |
|---|---|---|---|
| | | | and calculated as the weighted average of all values assigned to the 1°x1° bin and for each layer; The weights used for the averaging are the reciprocal square of the total retrieval errors associated with the partial columns retrieved in each layer. |
| O3_total_column_averaging_kernel | $(mol.m^{-2})$ / $(mol.m^{-2})$ | Nlat x Nlon x Nlayers | Merged ozone total column averaging kernel $((mole/m^2)/(mole/m^2))$ associated with the merged ozone partial column vertical profile, corresponding to the layers defined by the levels given in the variable atmosphere_pressure_grid and calculated as the weighted average of all values assigned to the 1°x1° bin and for each layer; The weights used for the averaging are the reciprocal square of the total retrieval errors associated with the partial columns retrieved in each layer. |

## *3.7. High-resolution Gap-free Merged Ozone Profile (Level-3) (FMI)*

### 3.7.1. Input data and algorithm

The high-resolution merged dataset of ozone profiles, LIMB-HIRES, is derived from a combination of ozone profiles from several satellite instruments in limb-viewing geometry. The first step of data processing is data homogenization, which includes the removal of biases and a-posteriori estimation of random uncertainties, thus making the data from different instruments compatible with each other. The high horizontal and vertical resolution dataset of ozone profiles is created via interpolation of the limb profiles from each day to 1°x1° horizonal grid. For the interpolation, a kriging-type interpolation method, which takes into account data uncertainties and the information about natural ozone variations from the SILAM-adjusted ozone field, is used. To mitigate the limited accuracy and coverage of the limb profile data in the UTLS, a smooth transition to the model data is applied below the tropopause. The details of data processing can be found in the ATBD and in Sofieva et al. (2022).

LIMB-HIRES covers the time period from 2004 to 2022. In the data files, both satellite interpolated ozone profiles and the profiles extended to troposphere using SILAM data, are included.

### 3.7.2. Parameters

The LIMB-HIRES data are collected in daily netCDF-4 file. For example, the file ESACCI-OZONE-L3-LP-LIMB_HIRES-20180901-fv0001.nc is for 1 September 2018. The main variables included in netCDF files are collected in Table 3.8.1.

**Table 3.8.1: The variables in LIMB-HIRES netCDF file. Npres, Nlat , Nlon are number of pressure levels, latitude and longitude zones, respectively.**

| Parameter | Unit | Dimensions | Description |
|---|---|---|---|
| pressure_ext | hPa | $N_{pres\_ext}\times 1$ | pressure levels for extended to troposphere data |
| pressure_sat | hPa | $N_{pres\_sat}\times 1$ | pressure levels for satellite data |
| latitude | degrees_north | $N_{lat}\times 1$ | Centers of latitude bins |
| longitude | degree_east | $N_{lon}\times 1$ | Centers of longitude bins |
| ozone_extended | $mol.m^{-3}$ | $N_{lat}\times N_{lon}\times N_{pres\_ext}$ | interpolated ozone profiles from satellites with extension to troposphere using SILAM data |
| ozone_extended_error | $mol.m^{-3}$ | $N_{lat}\times N_{lon}\times N_{pres\_ext}$ | random uncertainty of interpolated ozone profiles from satellites with extension to troposphere using SILAM data |
| ozone_satellite | $mol.m^{-3}$ | $N_{lat}\times N_{lon}\times N_{pres\_sat}$ | interpolated ozone profiles from satellites |
| ozone_satellite_error | $mol.m^{-3}$ | $N_{lat}\times N_{lon}\times N_{pres\_sat}$ | random uncertainty of interpolated ozone profiles from satellites |

## *3.8. OMPS-LP NOAA-21 Ozone Profile (Level-2) (IUP-UB)*

The UBR OMPS-LP L2 Ozone v1.0 product provides ozone profile retrieved at the University of Bremen (IUP-UB) for the central slit of the OMPS-LP instrument on the NOAA-21 (N21) satellite. The implemented retrieval approach for these observations is identical to the one applied to observations from the Suomi-NPP OMPS instrument. Ozone is retrieved by fitting sun-normalized radiance in four spectral windows, from 8.5 to 60.5 km on a 1 km grid and with a vertical resolution of approximately 2-3 km.

Retrieval for each observation state is performed independently. Spatial coverage is global (-82 to +82 degrees latitude), and there are about 14.5 orbits per day; each of them has typically 160 profiles with an along orbital track sampling of about 200 km.

### 3.8.1. Input data and algorithm

OMPS-LP L1G v2.6 are processed using SCIATRAN, the one-dimensional retrieval algorithm developed at IUP-UB.

### 3.8.2. Parameters

**Table 3.9.1: List of variables in the netCDF files**

| Parameter | Unit | Dimension | Description |
|---|---|---|---|
| time | days since 1900-01-01 00:00:00 | $N_{prof} \times 1$ | The parameter to index the profiles |
| altitude | km | $N_{alt} \times N_{prof}$ | The geometric altitude above the mean sea-level |
| pressure | hPa | $N_{alt} \times N_{prof}$ | Air pressure from ERA5 |
| latitude | degree_north | $N_{prof} \times 1$ | Latitude of each profile |
| longitude | degree_east | $N_{prof} \times 1$ | Longitude of each profile |

| Parameter | Unit | Dimension | Description |
|---|---|---|---|
| ozone_concentration | mol $m^{-3}$ | $N_{alt} \times N_{prof}$ | Vertical profiles of ozone. Number density ($cm^{-3}$) is acquired by multiplying the the factor NA=6.02214e17 $mol^{-1}$ |
| ozone_concentration_standard_error | mol $m^{-3}$ | $N_{alt} \times N_{prof}$ | Uncertainty (random error) associated with the ozone profiles |
| vertical_resolution | km | $N_{alt} \times N_{prof}$ | Vertical resolution for each profile |
| temperature_ecmwf | K | $N_{alt} \times N_{prof}$ | Temperature profiles at the locations of measurements from ERA5 |
| tropopause_altitude | km | $N_{prof} \times 1$ | Thermal tropopause altitude at the tangent point location computed from ERA5 temperature profile. |
| stratospheric_ozone_column | mol $m^{-2}$ | $N_{prof} \times 1$ | Integrated stratospheric profile from tropopause height to 60 km |

# 4. Using the data

## *4.1. Multi-Sensor Reanalysis 2 (Level-4) (KNMI)*

### 4.1.1. Data access and format

Besides at the Ozone_cci website, the MSR data set can be downloaded in a single netCDF data file C3S_TC_MSR2.nc via http://temis.nl/protocols/o3field/data/multimission/MSR-2.nc

### 4.1.2. Data reading examples (IDL, Matlab, Python)

Files may be read with standard NetCDF routines.

### 4.1.3. Preliminary evaluation

Uncertainties are provided per grid cell in the data file. A limited evaluation is given in van der A et al. (2015). Ground-based validation results can be consulted in the Product Validation and Intercomparison Report (PVIR v5.0, https://climate.esa.int/en/projects/ozone/key-documents).

### 4.1.4. Contacts

- Ronald van der A: ronald.van.der.a@knmi.nl
- Jos de Laat: laatdej@knmi.nl

## *4.2. Tropical Tropospheric Ozone CCD (Level-3) (DLR)*

### 4.2.1. Data access and format

The data are stored in netCDF file format and self explaining, they can be accessed via the CCI+ data server at BIRA.

### 4.2.2. Data reading examples (IDL, Matlab, Python)

Python example of a basic reading routine.

```
def read_month(s_path_to_file):
    ‘’’s_path_to file is the filename including the respective path
    returns two arrays for tropospheric columns and mixingratios
    qa values and errors might be added to the example’’’

    from netCDF4 import Dataset
    import numpy as np

    nc_in= Dataset(s_path_to_file,'r')

    trop_m=nc_in.variables['tropospheric_ozone_column']
    trop_s=nc_in.groups['SUPPORT_DATA'].groups['DETAILED_RESULTS']
        .variables['tropospheric_ozone_column sensors']
    trop_add=nc_in.groups['SUPPORT_DATA'].groups['DETAILED_RESULTS']
        .variables['tropospheric_ozone_column harmonisation sensors'][:]
    tropmr_m=nc_in.variables['tropospheric_ozone_mixingratio']
    tropmr_s=nc_in.groups['SUPPORT_DATA'].groups['DETAILED_RESULTS']
        .variables['tropospheric_ozone_mixingratio sensors']

    fa_trop_s=(trop_s[:]+trop_add[:,:,np.newaxis,np.newaxis]
        *np.ones_like(trop_s[:]))

    fa_tropold=np.ma.masked_values(trop_s[:],f_fillvalue)
    fa_corrfactor=fa_trop_s/fa_tropold
    fa_corrfactor=np.ma.mean(fa_corrfactor,axis=(2,3))
    fa_corrfactor=fa_corrfactor[:,:,np.newaxis,np.newaxis]
    fa_tropmr_s=tropmr_s[:]*fa_corrfactor  ## scale to include tropadd

    nc_in.close()

    fa_trop_m = fa_trop_m[:,np.newaxis,:,:]  ## columns
    fa_trop_r = np.ma.concatenate((fa_trop_s,fa_trop_m),axis=1)

    fa_tropmr_m = fa_tropmr_m[:,np.newaxis,:,:] ## mixing ratios
    fa_tropmr_r = np.ma.concatenate((fa_tropmr_s,fa_tropmr_m),axis=1)

    fa_tropmr_r=np.ma.masked_less(fa_tropmr_r,-990)
    np.ma.set_fill_value(fa_tropmr_r, f_fillvalue)

    return(fa_trop_r,fa_tropmr_r)
```

#### 4.2.3. Preliminary evaluation

An evaluation can be found in the Product Validation and Intercomparison Report (PVIR v5.0, https://climate.esa.int/en/projects/ozone/key-documents).

#### 4.2.4. Contacts

- Klaus-Peter Heue: Klaus-Peter.Heue@dlr.de

### *4.3. Limb-Nadir matched Tropospheric Ozone (Level-3) (FMI)*

#### 4.3.1. Data access and format

#### 4.3.2. Data reading examples (IDL, Matlab, Python)

NetCDF files can be read with various software such as Python, IDL, Matlab.

#### 4.3.3. Preliminary evaluation

An evaluation can be found in the Product Validation and Intercomparison Report (PVIR v5.0, https://climate.esa.int/en/projects/ozone/key-documents).

#### 4.3.4. Contacts

- Viktoria Sofieva: viktoria.sofieva@fmi.fi

### *4.4. UV-visible Merged Ozone Profile (Level-3) (DLR)*

#### 4.4.1. Data access and format

The Level-3 merged ozone profile product GOP-ECV is provided as netCDF files (one file per month). The content of the netCDF files is listed in Table 3.5.2 (see Sec. 3.5.2). The structure of the filenames is as follows: ESACCI-OZONE-L3S-NP-GOP_ECV-DLR_vzz_YYYYMM-fvxxxx.nc. zz denotes the algorithm version, YYYY denotes the year, MM is the month, and xxxx indicates the file version.

#### 4.4.2. Data reading examples (IDL, Matlab, Python)

Data reading example using Python. Table 3.5.2 (see Sec. 3.5.2) contains the complete list of variables in the netCDF file.

```
from netCDF4 import Dataset

filename = 'ESACCI-OZONE-L3S-NP-GOP_ECV-DLR_v02_202010-fv0200.nc'
ncfile = Dataset( filename, 'r' )

ozone_partial_column = ncfile.variables['ozone_partial_column’][:]
lat = ncfile.variables['latitude'][:]
lon = ncfile.variables['longitude'][:]

ncfile.close()
```

### 4.4.3. Preliminary evaluation

Ground-based validation results can be consulted in the Product Validation and Intercomparison Report (PVIR v5.0, https://climate.esa.int/en/projects/ozone/key-documents).

### 4.4.4. Contacts

- Diego Loyola: Diego.Loyola@dlr.de
- Melanie Coldewey-Egbers: Melanie.Coldewey-Egbers@dlr.de

## *4.5. IASI Ozone Profile CDR (Level-2) (ULB)*

### 4.5.1. Data access and format

The Level 2 IASI ozone profile CDR product processed at EUMETSAT is reformatted by LATMOS as netCDF-4 files (one file per day). The content of the netCDF files is listed in Table 3.6.1.

The IASI $O_3$ CDR product filename is as follows:

IASI_METOP{*X*}_L2_O3_PROFILE_{*yyyymmdd*}_EUMETSAT_CDR_V{*version*}.nc

where *X* = A or ab, and *yyyymmdd* is the date of IASI measurements and *version*=the product version number.

### 4.5.2. Data reading examples (IDL, Matlab, Python)

The netcdf-4 files can be read with standard software packages. The parameters of the netCDF files are listed in Table 3.6.1.

### 4.5.3. Preliminary evaluation

The netCDF files contain a variable named "retrieval_quality_flag" which is a general quality flag assessing the quality of the IASI $O_3$ CDR product. This quality flag is defined as follows:

- retrieval_quality_flag=2 for the most reliable pixels (based on the cost function), not used for the moment
- retrieval_quality_flag=1 for the valuable pixels, based on the quality flags previously described for the ULB-LATMOS FORLI-v20151001 files in the Ozone_cci+_D4.2_PUG_V1.1 document, along with the following quality control criterium: ratio of the $O_3$ partial column from ground to 6 km to the total $O_3$ column higher or equal to 0.085; if retrieval_quality_flag=1 is used, it is also recommended to filter out all data associated with DOFS lower than 2.
- retrieval_quality_flag=0 for the remaining pixels that we recommend not to use

The operational IASI $O_3$ profile dataset obtained running FORLI-$O_3$ (v20151001) has been extensively validated (Boynard et al., 2018 and Keppens et al., 2018) and used in several scientific publications related to analyses of ozone trends (e.g. Wespes et al., 2019). The reprocessed IASI $O_3$ profile CDR dataset obtained with FORLI-$O_3$ (v20151001) is under validation in the frame of this project.

Ground-based validation results can also be consulted in the Product Validation and Intercomparison Report (PVIR v5.0, https://climate.esa.int/en/projects/ozone/key-documents).

### 4.5.4. Contacts

At ULB:

- Catherine Wespes: catherine.wespes@ulb.be
- Pierre-François Coheur : pierre.coheur@ulb.be

At LATMOS :

- Juliette Hadji-Lazaro: Juliette.Hadji-Lazaro@latmos.ipsl.fr
- Anne Boynard : anne.boynard@latmos.ipsl.fr
- Cathy Clerbaux: cathy.clerbaux@latmos.ipsl.fr

## *4.6. IASI Merged Ozone Profile (Level-3) (ULB)*

### 4.6.1. Data access and format

The Level 3 IASI merged ozone profile product processed at ULB is formatted as netcdf-4 files (one file per day). The content of the netCDF files is listed in Table 3.7.1.

The L3 IASI merged $O_3$ product filename is as follows:

IASI_FORLI_O3_MERGED_{*yyyymmdd*}_V{*version*}.nc

where *yyyymmdd* is the date of IASI measurements.

### 4.6.2. Data reading examples (IDL, Matlab, Python)

The netcdf-4 files can be read with standard software packages. The parameters of the netCDF files are listed in Table 3.7.1.

### 4.6.3. Preliminary evaluation

The L3 IASI merged O3 profile dataset is based on the latest version (v20191122) of original FORLI-$O_3$ datasets that have been extensively validated (Boynard et al., 2018 and Keppens et al., 2018) and used in several scientific publications related to analyses of ozone trends (e.g. Wespes et al., 2019).

The L3 IASI merged $O_3$ profile dataset obtained using the original FORLI-$O_3$ datasets (v20191122) from the three IASI sensors is under validation in the frame of the project.

The general retrieval quality flag as recommended for the use of the ULB-LATMOS FORLI-$O_3$ files and described in the Ozone_cci+_D4.2_PUG_V1.1 document (PUG, https://climate.esa.int/en/projects/ozone/key-documents) has been applied on the original FORLI-$O_3$ datasets before merging.

Ground-based validation results can also be consulted in the Product Validation and Intercomparison Report (PVIR v5.0, https://climate.esa.int/en/projects/ozone/key-documents).

### 4.6.4. Contacts

- Catherine Wespes: catherine.wespes@ulb.be

## *4.7. High-resolution Gap-free Merged Ozone Profile (Level-3) (FMI)*

### 4.7.1. Data access and format

The LIMB-HIRES data are collected in daily netCDF-4 file. An example of file name is: ESACCI-OZONE-L3-LP-LIMB_HIRES-20180901-fv0001.nc for 1 September 2018.

### 4.7.2. Data reading examples (IDL, Matlab, Python)

NetCDF files can be read with various software such as Python, IDL, Matlab.

### 4.7.3. Preliminary evaluation

Ground-based validation results can be consulted in the Product Validation and Intercomparison Report (PVIR v5.0, https://climate.esa.int/en/projects/ozone/key-documents).

### 4.7.4. Contacts

- Viktoria Sofieva: viktoria.sofieva@fmi.fi

## *4.8. OMPS-LP NOAA-21 Ozone Profile (Level-2) (IUP-UB)*

### 4.8.1. Data access and format

OMPS-LP NOAA-21 retrieved at the IUP-UB have been converted to the HARMOZ format, with altitude vertical grid. These are monthly data files with self-explanatory names: e.g. ESACCI-OZONE-L2-LP-OMPS_N21-UBR-HARMOZ_ALT-YYYYMM-fvZZZZ.nc, where L2=Level 2, LP= Limb Profile, N21=NOAA-21, YYYY= year, MM=month, ZZZZ=file version.

### 4.8.2. Data reading examples (IDL, Matlab, Python)

Files are written in netCDF format, which can be read with standard routines (e.g. h5py and xarray in Python).

### 4.8.3. Preliminary evaluation

A preliminary evaluation of the retrieved profiles covering the year 2023 was performed by using Aura-MLS as a reference. In particular, differences between OMPS and collocated MLS profiles were evaluated. Relative differences are generally within ± 10% between 20 and 50 km and in the [60°S, 60°N] latitude range. Larger deviations were found below 20 km, especially in the tropics.

Ground-based validation results can be consulted in the Product Validation and Intercomparison Report (PVIR v5.0, https://climate.esa.int/en/projects/ozone/key-documents).

### 4.8.4. Contacts

- Carlo Arosio: carloarosio@iup.physik.uni-bremen.de

# 5. Acronyms, abbreviations and definition

| Acronym | Definition |
|---|---|
| ATBD | Algorithm Theoretical Basis Document |
| BIRA-IASB | Royal Belgian Institute for Space Aeronomy |
| CCI | Climate Change Initiative |
| CDR | Climate Data Record |
| CF | Climate Forecast (Conventions and Metadata) |
| DLR | German Aerospace Centre |
| DU | Dobson unit |
| ECMWF | European Centre for Medium-Range Weather Forecasts |
| ECV | Essential Climate Variable |
| ENVISAT | Environmental Satellite (ESA) |
| EO | Earth Observation |
| EOS | Earth Observing System |
| ERS | European Remote-Sensing Satellite |
| ESA | European Space Agency |
| EU | European Union |
| EUMETSAT | European Organisation for the Exploitation of Meteorological Satellites |
| FMI | Finnish Meteorological Institute |
| FORLI | Fast Optimal/Operational Retrieval on Layers for IASI |
| GCOS | Global Climate Observation System |
| GDP | GOME Data Processor |
| GODFIT | GOME-type direct-fitting retrieval algorithm |
| GOME | Global Ozone Monitoring Experiment (aboard ERS-2) |
| GOME-2 | Global Ozone Monitoring Experiment – 2 (aboard Metop-A) |
| GOP | GOME-type Ozone Profile |
| GTO | GOME-type Total Ozone |
| IASI | Infrared Atmospheric Sounding Interferometer |
| IR | Infra-Red |
| IUP | Institute of Environmental Physics, University of Bremen |
| ICDR | Intermediate Climate Data Record |
| KNMI | Royal Netherlands Meteorological Institute |
| LS | Low Stratosphere |
| LUT | Look-up table |
| Metop | Meteorological Operational Platform (EUMETSAT) |

| Acronym | Definition |
|---|---|
| MLS | Microwave Limb Sounder |
| MSR | Multi-Sensor Reanalysis |
| NetCDF | Network Common Data Form (data file format) |
| NOAA | US National Oceanic and Atmospheric Administration |
| NPP | Suomi National Polar-orbiting Partnership (NOAA / NASA / DoD) |
| $O_3$ | Ozone |
| OMI | Ozone Monitoring Instrument (aboard EOS-Aura) |
| OMPS | Ozone Mapping and Profiler Suite |
| PUG | Product User Guide |
| RAL | Rutherford Appleton Laboratory |
| RMS | Root mean square |
| RT | Radiative transfer |
| SBUV | Solar Backscatter Ultraviolet Radiometer |
| SCIAMACHY | Scanning Imaging Absorption Spectrometer for Atmospheric CHartographY (aboard Envisat) |
| SZA | Solar Zenith Angle |
| TROPOMI | TROPOspheric Monitoring Instrument |
| TOA | Top of the atmosphere |
| TOMS | Total Ozone Mapping Spectrometer |
| TP | Tropopause |
| UiB | Universität Bremen |
| ULB | Université libre de Bruxelles |
| UV | Ultraviolet |
| UV-Vis | Ultraviolet and visible light |
| WOUDC | World Ozone and Ultraviolet Radiation Data Centre |

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