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1. Purpose and scope

The Product User Guideline (PUG) is a deliverable of the ESA Ozone_cci+ project (http://www.esa-ozone-cci.org/). The Ozone_cci+ project will deliver the Essential Climate Variable (ECV) Ozone 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+, including a detailed description of the file format.

2. Overview of Ozone_cci+ products

The Ozone_cci+ includes data products for total ozone columns, ozone profiles from nadir sensors and stratospheric ozone profiles from limb and occultation sensors (Table 2.1). All data sets are reported in NetCDF-4 CF format following CCI and GCOS standards, and are freely available on the Ozone_cci web site (http://www.esa-ozone-cci.org/?q=node/160).

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

Product identifier	Source/ Processing center	Time periods	Altitude range	Spatial resolution	Temporal resolution	Uncertainty
Level-2 Data Sets						
TC_L2_GOME	BIRA	06/1995→ 07/2011	Total Column	320x40km²	3 days until Jun. 2003	<3%
TC_L2_SCIA	BIRA	08/2002 → 04/2012	Total Column	30x60km²	6 days	<3%
TC_L2_GOME2A	BIRA	01/2007 →	Total Column	80x40 km² (until Jul. 2013)	1.5 day	<3%
TC_L2_GOME2B	BIRA	01/2013 →	Total Column	80x40 km²	1.5 day	<3%
TC_L2_GOME2C	BIRA	01/2019 →	Total Column	80x40 km²	1.5 day	<3%
TC_L2_OMI	BIRA	10/2004 →	Total Column	13x24 km² at nadir)	1 day	<3%
TC_L2_OMPS	BIRA	02/2012 →	Total Column	50x50 km² at nadir)	1 day	<3%
TC_L2_TROPOMI	ESA	05/2018 →	Total Column	7x3.5 km² until Aug. 2019 5.5x3.5 km² after Aug. 2019	1 day	<3%
NP_L2_GOME	RAL	06/1995→ 07/2011	Ground to 80km (4-6km levels)	320x40km	Daily (morning overpass time)	Variable with latitude and season (usually <10% in the stratosphere and <40% in the troposphere

NP_L2_SCIA	RAL	08/2002 → 04/2012	Ground to 80km (4-6km levels)	240x30km	Daily (morning overpass time)	Variable with latitude and season (usually <10% in the stratosphere and <40% in the troposphere
NP_L2_OMI	RAL	10/2004 →	Ground to 80km (4-6km levels)	48x52km	Daily (afternoon overpass time)	Variable with latitude and season (usually <10% in the stratosphere and <40% in the troposphere
NP_L2_GOME2-A	RAL	01/2007 →	Ground to 80km (4-6km levels)	160x160km then 80x160km after 15th July 20213 (Tandem operation with GOME2-B)	Daily (morning overpass time)	Variable with latitude and season (usually <10% in the stratosphere and <40% in the troposphere
NP_L2_GOME2-B	RAL	01/2013 →	Ground to 80km (4-6km levels)	160x160km	Daily (morning overpass time)	Variable with latitude and season (usually <10% in the stratosphere and <40% in the troposphere
NP_L2_GOME2-C	RAL	01/2019 →	Ground to 80km (4-6km levels)	160x160km	Daily (morning overpass time)	TBD
NP_L2_IAS-A	ULB	10/2007 →	Ground to 60 km	IASI pixel (4 observations with a footprint of 12 km every 50 km)	Bi-daily (morning and afternoon overpass times)	Variable with latitude and season (usually <5% in the stratosphere and ~10-30% in the troposphere
NP_L2_IASI-B	ULB	05/2013 →	Ground to 60 km	IASI pixel (4 observations with a footprint of 12 km every 50 km)	Bi-daily (morning and afternoon overpass times)	Variable with latitude and season (usually <5% in the stratosphere and ~10-30% in

						the troposphere
NP_L2_IASI-C	ULB	09/2019 →	Ground to 60 km	IASI pixel (4 observations with a footprint of 12 km every 50 km)	Bi-daily (morning and afternoon overpass times)	Variable with latitude and season (usually <5% in the stratosphere and ~10-30% in the troposphere
NP_L2_OMI	BIRA	10/2004 →				
LP_L2_SCIA	UBR	08/2002 → 03/2012	8 65 km	3 - 5 km vertically and ~240 km along track	3 days	< 5 % middle stratosphere
LP_L2_MIPAS	KIT	07/2002 → 04/2012	6 -70 km	3 – 5 km	3 days	1-4 %
LP_L2_GOMOS	ESA	08/2002 → 12/2011	15 -90 km	2-3 km	Few weeks	0.5 – 5 %
LP_L2_SAGE2		10/1984 → 08/2005			1-2 months	
LP_L2_MLS		08/2004 →	261 - 0.02 hPa	2.5 – 4 km vertically	1 day	<5% between 2 and 68 hPa
LP_L2_SABER		01/2002 →			Few days; 2 months to get full latitude coverage	
LP_L2_HALOE		10/1991 → 09/2005			1-2 months	
LP_L2_OSIRIS	USask	11/2001 →	10 -60 km	~2 km	Few days	3-4 % middle stratosphere
LP_L2_SMR	CHALM	07/2001 → 08/2014	12 - 60 km	2.5 -3.5 km	Few weeks	~20%
LP_L2_ACE	UofT	02/2004 →	10 - 95 km	3-4 km vertically	Few months	<3% between 12-65 km
LP_L2_OMPS	Usask	02/2012 →	10 – 60 km	1-2 km vertically, 300-400 km horizontally	3-4 days	2-5 %
Level-3 Data Sets						
TC_L3_MRG	DLR/BIRA	07/1995 → 12/2020	Total Column	1° x 1°	1 month	<3%
NP_L3_MRG	RAL/KNMI/DLR	07/1995 →	See e.g. NP_L2_GOME	tbd	1 month	tbd
LP_L3_SCIA	FMI	TBD/TBC	TBD/TBC	TBD/TBC	TBD/TBC	TBD/TBC
LP_L3_MIPAS	FMI	TBD/TBC	TBD/TBC	TBD/TBC	TBD/TBC	TBD/TBC
LP_L3_GOMOS	FMI	TBD/TBC	TBD/TBC	TBD/TBC	TBD/TBC	TBD/TBC
LP_L3_OSIRIS	FMI	TBD/TBC	TBD/TBC	TBD/TBC	TBD/TBC	TBD/TBC
LP_L3_SMR	CHALM	TBD/TBC	TBD/TBC	TBD/TBC	TBD/TBC	TBD/TBC
LP_L3_ACE	FMI	TBD/TBC	TBD/TBC	TBD/TBC	TBD/TBC	TBD/TBC
LP_L3_MRG-MZM	FMI	TBD/TBC	TBD/TBC	TBD/TBC	TBD/TBC	TBD/TBC

LP_L3_MRG-Latlon	FMI	TBD/TBC	TBD/TBC	TBD/TBC	TBD/TBC	TBD/TBC
Level-4 Data Sets						
NP_L4_MSR	KNMI	1957-2020	Total column	0.5 º x0.5 º	monthly	Variable

On total ozone, 25 years of harmonized level-2 data records from GOME, SCIAMACHY, GOME-2A, GOME-2B, GOME-2C, OMI and OMPS sensors have been produced using an advanced version of the direct-fitting GODFIT-4 prototype algorithm. In addition, the TROPOMI operational offline total ozone product is also based on GODFIT-4 and shows a high level of consistency with the other sensors. This data set includes the Level 2 products for each instrument (over full instrument lifetime). From the level-2 data records the corresponding level-3 data records have been computed as 1°x1° gridded monthly means. Additionally a merged data set including all individual level-3 data records has been generated. OMI is used as a long-term stability reference in order to homogenize the individual records before the merging.

For ozone profiles, data set from GOME (for the year 1997) and GOME-2 (for the years 2007-2008) instruments have been generated. Beside the level 2 data sets for the GOME and GOME-2 instruments, monthly mean gridded and assimilated 6 hourly global ozone fields are provided. Level 2 datasets from IASI/Metop-A (from 2007 to now), -B (from 2012 to now) and -C (from 2018 to now) are produced and available on the French AERIS database (https://iasi.aeris-data.fr/catalog/). The datasets include ozone profiles along with corresponding averaging kernels and relative total error profile, on the same vertical grid, meeting a series of quality control criteria.

As regards limb sensors, the so-called Harmonized single instruments (HARMOZ) data sets has been generated for the GOMOS, MIPAS, SCIAMACHY, OSIRIS, SMR and ACE-FTS instruments. These data records (covering instrument lifetime except for MIPAS – after 2005 only) include individual profiles with a common pressure grid and concentration unit, auxiliary information for converting into mixing ratio and/or geometric altitude. In addition, for each pair of instruments, drift and bias tables are provided. Beside the single profile data, single instrument zonal mean time series (10° latitude bin) including detailed uncertainty/variability information are also available.

Merged ozone profile data sets covering two contiguous years (2007-2008) have been created from all limb/occultation sensors onboard of ENVISAT (GOMOS, MIPAS, SCIAMACHY) as well as from the Third Party Missions OSIRIS, SMR and ACE-FTS. The merged data sets include monthly zonal mean and bi-weekly mean (20° longitude, 10° latitude, monthly) ozone profiles.

3. Data processing and parameters

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

3.1. L2 Total Ozone (BIRA-IASB)

3.1.1. Input data and algorithm

3.1.1.1. Algorithm

Level-2 total ozone column data sets derived from the sensors GOME/ERS-2, SCIAMACHY/ENVISAT, GOME-2/METOP-A, GOME-2/METOP-B, GOME-2/METOP-C, OMI/AURA and OMPS-NM/Suomi-NPP have been processed with the retrieval algorithm GODFIT v4 developed at BIRA-IASB. The data sets are provided for the complete instrumental time series, under the condition of availability of the input parameters, and are based on the latest level-1 available data. This ensemble of products is complemented by the operational TROPOMI total ozone offline product, which is based on GODFIT and consequently provides consistent retrievals. For further description of the latter product, the reader is invited to refer to documentation available at http://www.tropomi.eu/data-products/total-ozone-column (ATBD, PUM, README).

The GOME-type Direct Fitting (GODFIT) algorithm version 4 relies on a direct-fitting approach to retrieve in a one-single step total ozone columns from satellite nadir UV hyperspectral measurements. A non-linear least squares minimization of differences between measured and simulated reflectances is performed in the Huggins bands (fitting window: 325-335 nm) which provides high sensitivity to ozone absorption down to the surface. In addition to total ozone, a number of other parameters form the state vector, including the effective temperature, an effective albedo for the observed scene, and the amplitude of the inelastic structures (Ring effect). Simulations are performed on the fly with the radiative transfer model LIDORT, which also provides the Jacobians required for the inversion. Alternatively, in order to further accelerate the retrievals, the simulated data can be extracted from precomputed look-up tables, e.g. for sensors providing large amount of data.

One particular aspect of the CCI algorithm is that it includes an optional soft-calibration procedure of the L1b data, allowing to further reducing possible systematic biases in the L2 retrievals attributed to limitations in the L1 calibration. This procedure is currently applied to SCIAMACHY and GOME-2A and B. Thanks to the application of one common retrieval approach and to this soft-calibration procedure, it has been shown that all individual L2 data sets agree with ground-based reference measurements at the percent level (Garane et al., 2018, 2019). The high maturity of the total ozone L2 retrievals developed within CCI allows producing and extending operationally the different level-2 data sets as part of the Copernicus Climate Change Service (C3S) activities. Figure 3.1 illustrates the current total ozone time series obtained when the different data sets available are combined together. More details on the algorithm can be found in Lerot et al. (2014) and Garane et al. (2018).

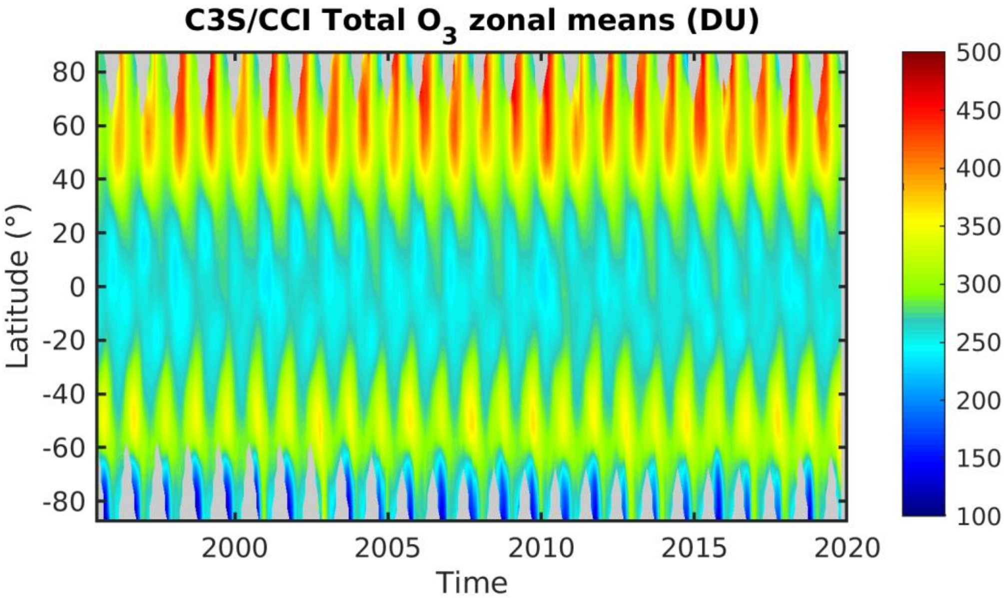

Figure 3.1: : Illustration of the total ozone time series as produced as part of the CCI and C3S activities and obtained by combining different sensors (GOME, SCIAMACHY, GOME-2A/B, OMI, OMPS).

3.1.1.2. Input data

A series of static and dynamic inputs are required to produce the CCI L2 data sets, as listed in Table 3.1 and 3.Table 3.2 While static input are common for all sensors, dynamic parameters need to be ingested from specific products. Static data include ozone cross-sections, reference high-resolution solar spectrum, surface albedo and altitude, and a database of a priori ozone vertical profile shape. Dynamic parameters include measured spectra and geolocations as part of the L1 products, as well as needed cloud parameters (cover and altitude) extracted from different products.

Table 3.1: List of static input

Parameter	Unit	Source
High-resolution solar spectrum	$mol.s^{-1}.m^{-2}.nm^{-1}$	Chance and Kurucz [2010]
Absorption O_3 cross sections	$cm^2 molec.^{-1}$	Serdyuchenko et al., 2014, pre-shifted by +0.0035 nm
Surface Albedo at 335 nm	---	OMI LER database (Kleipool et al. [2008])
Surface altitude	m	GMTED2010 (Danielson et al., 2011)
A-priori O_3 vertical profile shapes	vmr	Total O_3-classified climatology (Labow et al., [2015]) combined with the OMI/MLS tropospheric O_3 climatology (Ziemke et al., [2011])

Table 3.2: List of products required for dynamic inputs (L1 and cloud parameters)

Sensor	Level-1 data	Cloud Product
GOME/ERS-2	ESA L1 v4.00/4.01/4.03	FRESCOv7 (Wang et al., 2008)
SCIAMACHY/ENVISAT	ESA L1 v8.0x	FRESCOv7 (Wang et al., 2008)
GOME-2/METOP-A	EUMETSAT L1 v5.12/6.12	FRESCOv7 (Wang et al., 2008)
GOME-2/METOP-B	EUMETSAT L1 v5.12/6.12	FRESCOv7 (Wang et al., 2008)
GOME-2/METOP-C	EUMETSAT L1 v5.12/6.12	FRESCOv7 (Wang et al., 2008)
OMI/AURA	NASA Collection 3	OMCLDO2 (Veefkind et al., 2016)
OMPS/Suomi-NPP	NMEV-L1B v2/v2.1	NMTO3_L2.2 (Jaross et al., 2017)

3.1.2. Parameters

There is one ozone column measurement per ground pixel observed by the sensor and the level-2 data sets are distributed via Net-CDF files (one file per orbit). For each measurement, geolocation information, auxiliary and additional fitted parameters, quality indicators, a-priori O3 profile shape and averaging kernels are also provided in the output files. Figure 3.**2** shows an example of total ozone columns retrieved from one day of GOME-2/METOP-A observations.

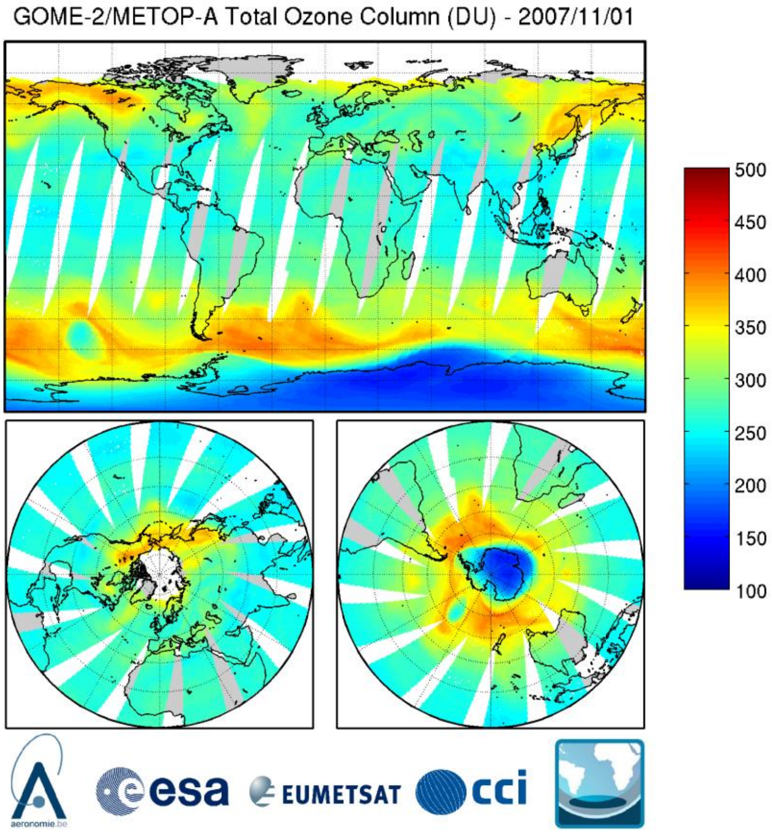

Figure 3.2: Total ozone columns retrieved from GOME-2/METOP-A observations on 1st November 2007

The delivered Net-CDF files contain only measurements for which the convergence has been reached with a number of iterations less than 6 (the typical number of iterations is 3-4). No retrieval is performed for pixels with solar zenith angle larger than 89°. The quality of the total ozone measurements following some specific instrumental operations (e.g. decontamination episodes) may be degraded. These measurements are in general easily detectable and have already been filtered out from the delivered level-2 data sets.
An estimation of the random error is associated to each total ozone column given in the product. This value has been derived via propagation of the level-1 radiance and irradiance statistical errors throughout the inversion algorithm. The reduced chi-squared value is a good indicator of the consistency between the fit residuals and the level-1 errors. Assuming perfectly estimated level-1 errors, the reduced chi-squared will be very close to 1 for a fit without any systematic structures in its residuals. In practice, they are generally ranging between 0.3 and 3. The root mean-squared (RMS) of the fit residuals is another indicator for the fit quality, but does not provide any hint on the nature of the residuals (random or systematic).
As mentioned before, the averaging kernels are also provided for all measurements. They represent the sensitivity of the total column retrieval to a real change in the ozone concentration at a given layer, considering both the observation geometry and the algorithmic features. At low and mid-latitudes, these averaging kernels are generally close to 1 in the stratosphere and upper troposphere and decrease for the lowermost layers, depending on the surface albedo and cloud contamination. At higher solar zenith angles, they change more rapidly with the altitude, making the retrieval quality much more dependent on the a priori profile shape information. Typical averaging kernels are illustrated in Figure 3.3 for one GOME orbit. The black dots represent the pressure of the effective scene considered for the total ozone retrieval. A smoothing error

estimate is also provided in the level-2 files, which represents the impact of the a priori profiles shape on the retrieved column. This is computed using both the averaging kernel and the covariance matrices associated to the a priori profile climatology.
These different parameters can be used by the user to apply additional filtering for an optimal use of these data sets adapted to its own application. Although the total error on the individual measurements is generally within a few percent, it can be much larger in some specific geophysical conditions unaccounted for in the retrieval algorithm like the presence of large aerosol plumes or major volcanic eruptions leading to clouds of SO2 and ashes.

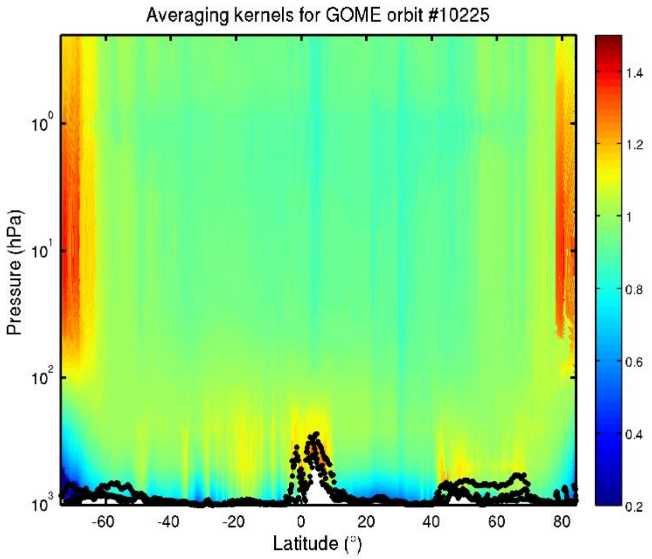

Figure 3.3: Typical averaging kernels of total ozone retrievals for one GOME orbit. The black dots represent the pressure of the effective scenes considered

Table 3.3.3 below describes all variables contained in the level-2 total ozone output NetCDF files in a plain structure.

Table 3.3: Dimension and description of all variables contained in the L2 total ozone NetCDF files. N_p represents the total number of measurements for scanning instruments (GOME, SCIAMACHY, GOME-2) and the number of viewing lines for imager instruments (OMI, OMPS). N_r is the number of rows for imager instruments (60 for OMI, 30 for OMPS), and is 1 for scanner instruments. N_{sw} is the number of subwindows used in the wavelength calibration procedure applied once per orbit and N_{cal} is the number of fitted parameters during this procedure.

Parameter	Unit	Dimension	Description
Time	days	$N_p \times N_r$	Time of measurement in days since 1995-1-1 00:00:00
time_of_measurement_string	-	$N_p \times N_r \times 19$	String indicating the time of measurement at a glance: YYYYMMDDThhmmss.sss
pixel_number	-	$N_p \times N_r$	Ground pixel number
state_number	-	$N_p \times N_r$	State/MDR/Viewing line number. Only relevant for SCIAMACHY, GOME-2 and OMI.
row_number	-	$N_p \times N_r$	Row index number. Only relevant for OMI.
pixel_type	-	$N_p \times N_r$	Pixel type: 0 for forward pixels, 3 for backscan pixels, -1: NA
Latitude	degree	$N_p \times N_r$	Latitude of the pixel center
latitude_corner	degree	$4 \times N_p \times N_r$	Latitudes of the pixel corners

Longitude	degree	$N_p \times N_r$	Longitude of the pixel center
longitude_corner	degree	$4 \times N_p \times N_r$	Longitudes of the pixel corners
solar_zenith_angle	degree	$N_p \times N_r$	Solar zenith angle at the pixel center
viewing_zenith_angle	degree	$N_p \times N_r$	Viewing zenith angle at the pixel center.
relative_azimuth_angle	degree	$N_p \times N_r$	Relative azimuth angle at the pixel center
retrieval_mode_flags	-	$N_p \times N_r$	retrieval mode: 0 for normal mode, 1 for snow/ice mode from cloud algorithm
processing_flags	-	$N_p \times N_r$	0: Nominal mode; 1: irregular L1 data - No retrieval; 2: Solar zenith angle larger than 89° - No retrieval; 3: No cloud data - No retrieval; 8: Forward model failure - No retrieval; 9: inversion failure - No retrieval; 21: Pixel affected by row anomaly - No retrieval; 22-24: Pixel might be affected by row anomaly - uncertain output
Total_ozone_column	$mol.m^{-2}$	$N_p \times N_r$	Retrieved total ozone column
Total_ozone_column_ random_error	$mol.m^{-2}$	$N_p \times N_r$	Random error associated to the retrieved total column
Total_ozone_column_ smoothing_error	$mol.m^{-2}$	$N_p \times N_r$	Error due to the a priori profile associated to the retrieved total column
ozone_ghost_column	$mol.m^{-2}$	$N_p \times N_r$	Partial ozone column comprised between the ground and the effective surface
fitted_ring_coefficient	-	$N_p \times N_r$	Retrieved Ring scaling parameter
fitted_state_vector	Various	$8 \times N_p \times N_r$	Full fitted state vector (Total O3, T°-shift, 4 polynomial coefficients, Ring scale factor, Radiance wavelength shift)
effective_temperature	°K	$N_p \times N_r$	Retrieved effective temperature
cloud_fraction	-	$N_p \times N_r$	Effective cloud fraction
cloud_top_pressure	hPa	$N_p \times N_r$	Cloud Top pressure
cloud_albedo	-	$N_p \times N_r$	Effective cloud top albedo provided by
effective_scene_pressure	hPa	$N_p \times N_r$	Pressure at the effective scene used for the retrieval
effective_scene_albedo	-	$N_p \times N_r$	Retrieved effective albedo of the scene
surface albedo	-	$N_p \times N_r$	Minimum surface albedo at 335 nm from OMI LER climatology
surface_altitude	m	$N_p \times N_r$	Surface altitude extracted from GTOPO30
Rms	-	$N_p \times N_r$	Root mean square of fit residuals
reduced_chi_squared	-	$N_p \times N_r$	Reduced chi-square of the fit
nb_of_iterations	-	$N_p \times N_r$	Number of iterations before convergence
convergence_flag	-	$N_p \times N_r$	Convergence flag: 0 for failure, 1 for success
atmosphere_ pressure_grid	hPa	$15 \times N_p \times N_r$	Pressure at levels defining the layers used in the forward model
averaging_kernels	-	$14 \times N_p \times N_r$	Averaging kernels in the layers of the forward model
apriori_ozone_profile	mol.m-2	$14 \times N_p \times N_r$	A-priori partial ozone columns in the layers of the forward model

Wavelength_calibration_parameters	-	$N_{cal} \times N_{sw} \times N_r$	Wavelength calibration fitted parameters in each subwindow: 1 wavelength shift and optionally 1 or 2 slit function parameters.
Wavelength_calibration_rms	-	$N_{sw} \times N_r$	Root mean square of wavelength calibration fit residuals in each subwindow

3.2. L3 Total Ozone (DLR)

3.2.1. Input data and algorithm

The individual L2 total ozone data as described in Sec. 3.1 are used as input for the L3 processing. We use data from the satellite sensors GOME/ERS-2, SCIAMACHY/ENVISAT, OMI/Aura, GOME-2/MetOp-A, GOME-2/MetOp-B, and TROPOMI/S5P. They are mapped onto a regular global grid of 1°×1° in latitude and longitude to construct monthly averages for each sensor.

3.2.2. Parameters

The content of the L3 total ozone netCDF files per sensor is listed in Table 3.4.

Table 3.4: Variables in the monthly L3 total ozone netCDF files. N_{lat}=180 and N_{lon}=360

Parameter	Unit	Dimensions	Description
Latitude	degrees north	N_{lat}	Latitude of grid center
Longitude	degrees east	N_{lon}	Longitude of grid center
total_ozone_column	mol.m^{-2}	$N_{lat} \times N_{lon}$	Monthly mean otal ozone column
total_ozone_column_number_of_observations	-	$N_{lat} \times N_{lon}$	Number of observations per month
total_ozone_column_standard_deviation	mol.m^{-2}	$N_{lat} \times N_{lon}$	Standard devation of monthly mean total ozone column
total_ozone_column_standard_error	mol.m^{-2}	$N_{lat} \times N_{lon}$	Standard error of monthly mean total ozone column

3.3. L3 Merged Total Ozone (GTO-ECV) (DLR)

3.3.1. Input data and algorithm

The individual L3 total ozone data as described in Sec. 3.2 are used as input to construct the merged L3 total ozone product called GTO-ECV (GOME-type Total Ozone Essential Climate Variable). These products are combined into one single cohesive record. Before merging the individual data records, corrections are applied in order to account for possible remaining inter-sensor biases and drifts. Owing to its remarkable long-term stability with respect to the ground-based reference (Garane et al., 2018), the OMI record is used as a reference basis for GTO-ECV, while GOME, SCIAMACHY, GOME-2A, GOME-2B, and TROPOMI are adjusted in terms of correction factors that depend on latitude and time. A detailed description can be found in Coldewey-Egbers et al. (2015) and in Garane et al. (2018).

The product contains monthly mean ozone columns on a regular grid of 1°x1° in latitude and longitude.

3.3.2. Parameters

The content of the L3 merged total ozone GTO-ECV netCDF files is listed in Table 3.5.

Table 3.5: Variables in the merged monthly L3 total ozone netCDF files of the GTO-ECV product. N_{lat}=180 and N_{lon}=360.

Parameter	Unit	Dimension	Description
Latitude	degrees north	N_{lat}	Latitude of grid center
Longitude	degrees east	N_{lon}	Longitude of grid center
total_ozone_column	mol.m^{-2}	$N_{lat} \times N_{lon}$	Monthly mean total ozone column
total_ozone_column_number_of_observations	-	$N_{lat} \times N_{lat}$	Number of observations per month
total_ozone_column_standard_deviation	mol.m^{-2}	$N_{lat} \times N_{lat}$	Standard devation of monthly mean total ozone column
total_ozone_column_standard_error	mol.m^{-2}	$N_{lat} \times N_{lat}$	Standard error of monthly mean total ozone column

3.4. L4 Total Ozone Multi-Sensor Reanalysis (MSR) (KNMI)

3.4.1. 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 18 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, 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).

3.4.2. Parameters

In Tables 3.6 and 3.7 (meta data and data), the content of the data file is explained.

Table 3.6: 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
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 3.7: 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 1970
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	Dobson Unit	$N_{date} \times N_{alt} \times N_{lat}$	Merged deseasonalized anomalies, see [Sofieva et al., 2017] for details
Standard deviation of monthly average ozone column	Dobson Unit	$N_{date} \times N_{alt} \times N_{lat}$	Vertical profiles of merged monthly zonal mean ozone mole concentration.

3.5. L2 Nadir BUV Ozone Profile (RAL)

This describes the details of this particular ozone profile dataset, including pertinent attributes of the data and algorithm used. For a full technical description of the retrieval algorithm used please refer to the Ozone_cci ATBD.

3.5.1. Input data and algorithm

Table 3.8: List of level 1b inputs

Sensor	Time coverage	Level-1 data	RAL Algorithm (latest)
GOME/ERS-2	Jul. 1995 – Jun. 2011	ESA L1 v4.00/4.01/4.03	fv0301
SCIAMACHY/ENVISAT	Aug. 2002 – Apr. 2012	ESA L1 v7.04	fv0300
GOME-2/METOP-A	Jan. 2007 – current	EUMETSAT L1 v5.3-6.3	fv0300
GOME-2/METOP-B	Jan. 2013 – current	EUMETSAT L1 v5.3-6.3	v0215/fv0302
OMI/AURA	Oct. 2004 - current	NASA Collection 3	fv0214

3.5.2. Parameters

RAL L2 nadir profile data are stored in NetCDF files. Climate Forecast (CF) convention standard names are provided where applicable.

Table 3.9: List of variables in the NetCDF files

Parameter	Unit	Dimension	Description
o3_nd	cm^{-3}	$N_{prof} \times$ n_o3_nd	Ozone molecular number density
o3_vmr	-	$N_{prof} \times$ n_o3_vmr	Ozone volume mixing ratio
o3_error	%	$N_{prof} \times$ n_o3_error	Retrieved ozone uncertainty
o3_ap	-	$N_{prof} \times$ n_o3_ap	Ozone a priori volume mixing ratio
o3_ap_error	%	$N_{prof} \times$ n_o3_ap_error	Ozone a priori error
o3_sub_col	DU	$N_{prof} \times$ n_o3_sub_col	Ozone partial column
o3_sub_col_error	DU	$N_{prof} \times$ n_o3_sub_col_error	Ozone partial column error
o3_sub_col_sn	DU	$N_{prof} \times$ n_o3_sub_col_sn	Ozone partial column noise error
o3_ap_sub_col	DU	$N_{prof} \times$ n_o3_sub_col	Ozone a priori partial column
o3_ap_sub_col_error	DU	$N_{prof} \times$ n_o3_ap_sub_col	Ozone a priori partial column error
o3_ap_sub_col_model	DU	$N_{prof} \times$ n_o3_sub_col_model	Ozone a priori partial column on higher resolution true grid
o3_tc	DU	$N_{prof} \times 1$	Total column ozone
o3_tc_error	DU	$N_{prof} \times 1$	Total column ozone error
o3_tc_error_sn	DU	$N_{prof} \times 1$	Total column ozone noise error
o3_ap_tc_error	DU	$N_{prof} \times 1$	Ozone a priori total column error
o3_b1_sub_col	DU	$N_{prof} \times$ n_o3_b1_sub_col	Band 1 ozone partial column
o3_b1_sub_col_error	DU	$N_{prof} \times$ n_o3_b1_sub_col_error	Band 1 ozone partial column error
o3_b1_tc	DU	$N_{prof} \times 1$	Band 1 total ozone column
o3_b1_tc_error	DU	$N_{prof} \times 1$	Band 1 total ozone column error
Nit	-	$N_{prof} \times 1$	Number of Iterations
b1nit	-	$N_{prof} \times 1$	Band 1 number of iterations
Cost	-	$N_{prof} \times 1$	Final cost function value
Ncost	-	$N_{prof} \times 1$	Normalized final cost function value
b1cost	-	$N_{prof} \times 1$	Band 1 cost function value
Aconv	-	$N_{prof} \times 1$	Convergence flag
b1conv	-	$N_{prof} \times 1$	Band 1 convergence flag

Parameter	Unit	Dimension	Description
Achi	-	$N_{prof} \times 1$	Chi squared flag
b1fail	-	$N_{prof} \times 1$	B1 retrieval failure flag: 0=OK, 1=b1 not attempted, too many spikes, 2=b1 carried out but not used in b2 so reduced information content
Dofs	-	$N_{prof} \times 1$	Ozone degrees of freedom from signal
spres	hPa	$N_{prof} \times 1$	Surface Pressure
Levs	hPa	$N_{levels} \times 1$	Pressure levels of retrieved ozone profiles
o3_z	km	$N_{prof} \times$ n_o3_z	Altitude levels of retrieved ozone profiles
lat	degrees north	$N_{prof} \times 1$	Latitude of ground pixel center
Lon	degrees east	$N_{prof} \times 1$	Longitude of ground pixel center
ll	degrees north/degrees east	$N_{prof} \times 8$	Latitude and longitude of ground pixel corners. [lat1,lon1,lat2,lon2,lat3,lon3,lat4,lon4]
Pixno	-	$N_{prof} \times 1$	Orbit ground pixel number ([scan line number * 100]+cross track scan position index)
Sza	degrees	$N_{prof} \times 1$	Solar zenith angle
lza	degrees	$N_{prof} \times 1$	Line-of-sight zenith angle
saa ***	degrees	$N_{prof} \times 1$	Solar azimuth angle
laa ***	degrees	$N_{prof} \times 1$	Line-of-sight azimuth angle
time	hours	$N_{prof} \times 1$	Hours since 00:00.00hrs on date
Scp	-	$N_{prof} \times 1$	Across track scan index
Cloudf	-	$N_{prof} \times 1$	FRESCO effective cloud fraction
Cloudp	hPa	$N_{prof} \times 1$	FRESCO cloud top pressure
Clouda	-	$N_{prof} \times 1$	FRESCO cloud albedo
cloud_ffail	-	$N_{prof} \times 1$	FRESCO cloud fit fail indication
cloud_mode	-	$N_{prof} \times 1$	FRESCO cloud fit mode
cloud_s6	-	$N_{prof} \times 1$	Expected scaling of 0-6km sub column due to cloud
cloud_s12	-	$N_{prof} \times 1$	Expected scaling of 0-12km sub column due to cloud
Salb	-	$N_{prof} \times 1$	Retrieved surface albedo
salb_err	-	$N_{prof} \times 1$	Retrieved surface albedo error
Ring	-	$N_{prof} \times 1$	Retrieved ring spectrum scaling parameter
ring_err	-	$N_{prof} \times 1$	Retrieved ring spectrum scaling parameter error
Xsect	-	$N_{prof} \times 1$	Retrieved wavelength shift of absorptions cross sections
xsect_err	-	$N_{prof} \times 1$	Retrieved wavelength shift of absorptions cross sections error
Bro	-	$N_{prof} \times 1$	BrO column average volume mixing ratio
bro_err	-	$N_{prof} \times 1$	BrO column average volume mixing ratio error
no2	-	$N_{prof} \times 1$	NO_2 column average volume mixing ratio

Parameter	Unit	Dimension	Description
no2_err	-	$N_{prof} \times 1$	NO_2 column average volume mixing ratio error
ch2o	-	$N_{prof} \times 1$	CH_2O column average volume mixing ratio
ch2o_err	-	$N_{prof} \times 1$	CH_2O column average volume mixing ratio error
Rsf	-	$N_{prof} \times 1$	Residual spectral pattern scaling factor
rsf_err	-	$N_{prof} \times 1$	Residual spectral pattern scaling factor error
Slit	-	$N_{prof} \times 1$	Slit function FWHM scaling parameter
slit_err	-	$N_{prof} \times 1$	Slit function FWHM scaling parameter error
Misr	nm	$N_{prof} \times$ n_misr	Wavelength shift between radiance and irradiance spectra
misr_err	nm	$N_{prof} \times$ n_misr	Wavelength shift between radiance and irradiance spectra error
Gain	-	$N_{prof} \times$ n_gain	Radiometric scale factor polynomial coefficient
gain_err	-	$N_{prof} \times$ n_gain_err	Radiometric scale factor polynomial coefficient error
Offset	-	$N_{prof} \times$ n_offset	Radiometric offset polynomial coefficient
offset_err	-	$N_{prof} \times$ n_offset_err	Radiometric offset polynomial coefficient error
b1_leak **	-	$N_{prof} \times$ n_b1_leak	B1 radiometric offset parameter
b1_leak_err **	-	$N_{prof} \times$ n_b1_leak_err	B1 radiometric offset parameter error
b1_salb	-	$N_{prof} \times 1$	Retrieved surface albedo
b1_salb_err	-	$N_{prof} \times 1$	Retrieved surface albedo error
b1_ring	-	$N_{prof} \times$ n_b1_ring	Retrieved ring spectrum scaling parameter
b1_ring_err	-	$N_{prof} \times$ n_b1_ring	Retrieved ring spectrum scaling parameter error
b1_fcal	-	$N_{prof} \times 1$	B1 wavelength shift of sun normalized radiance
b1_fcal_err	-	$N_{prof} \times 1$	B1 wavelength shift of sun normalized radiance error
model_levs	-	n_model_levels	Pressure levels of higher res sub-column AKs for retrieved ozone profiles (ak_rsg_tsc)
fm_levs	km	$N_{prof} \times$ n_fm_levs	FM level height (Fixed 2km space)
fm_temperature	K	$N_{prof} \times$ n_fm_temperature	FM level temperature
fm_pressure	hPa	$N_{prof} \times$ n_fm_pressure	FM pressure profile
sx	cm^{-6}	$N_{prof} \times$ n_sx_1 $\times$ n_sx_0	Ozone molecular number density solution covariance matrix
Sn	cm^{-6}	$N_{prof} \times$ n_sx_1 $\times$ n_sx_0	Ozone molecular number density measurement noise covariance matrix
Ak	-	$N_{prof} \times$ n_ak_1 $\times$ n_ak_0	Ozone molecular number density averaging kernel matrix
ak_rsc_tsc #1	-	$N_{prof} \times$ n_ak_1 $\times$ n_ak_0	Ozone molecular number density averaging kernel matrix (Retrieved vs true sub-column). Preferred version.

Parameter	Unit	Dimension	Description
ak_sc_sc #2	-	$N_{prof} \times$ n_ak_1 × n_ak_0	Ozone molecular number density averaging kernel matrix (Use if ak_rsc_tsc not possible)
akh #3,*	-	$N_{prof} \times$ n_ak_1 × n_ak_0	Ozone molecular number density averaging kernel matrix
imak_apr_sc	DU	$N_{prof} \times$ n_imak_apr_sc	a priori contribution to estimated sub-column

Note : Some parameters added in later versions or instrument dependent (generally=1 if not specified) :

*=fv0300+

**=fv0301+ n_b1_leak & n_b1_leak_error

***=fv302+ saa & laa

Important note on AK :
#1 AK_RSC_TSC (Retrieved Sub Column vs True Sub Column). This version of the AK should be used whenever possible to reduce errors in representing FM assumptions on vertical interpolation of the profile in the lower atmosphere. See ATBD.
#2 AK_SC_SC This is the standard square Sub-Column vs Sub-Column AK for use if #1 really cannot be used. See ATBD.
#3 AKH For high resolution perturbations

3.6. L2 Nadir IASI Ozone Profile (ULB)

3.6.1. 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 O_3 product has been generated at ULB using the FORLI (Fast Optimal Retrieval on Layers for IASI) software (Hurtmans et al., 2012) in the framework of the Ozone_cci project. FORLI relies on a fast radiative transfer and retrieval methodology based on the Optimal Estimation Method (Rodgers, 2000).

The dataset is provided for the period 2008 - present for the three IASI instruments (IASI-A, -B and -C). The FORLI algorithm operates with multiplication factors, with the a priori as reference, and the profile is adjusted in layer partial columns. The IASI O_3 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 relative total error profile, on the same vertical grid.

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 current database is generated from IASI ozone retrievals processed at ULB-LATMOS using FORLI software v20151001 up to 11 December 2019 and using FORLI software v20191122 up to 26 February 2020. The current database is not updated after this date.
Indeed, the FORLI software v20151001 (Hurtmans et al., 2012) was implemented at EUMETSAT in 2019 and the IASI O_3 product is operational at EUMETSAT and distributed via Eumetcast in BUFR format since 4 December 2019. The Eumetsat IASI O3 BUFR files are reformatted in netcdf format by LATMOS and are now distributed by AERIS. They constitute the new CCI database from 4 December 2019. Hence, we recommend to use the ULB-LATMOS FORLI-v20151001 dataset from 20071001 to 20191204 and the EUMETSAT FORLI-v20151001 dataset afterwards, both being available on the AERIS database.

3.6.2. Parameters

Tables 3.10a and b describe the variables contained in the ULB-LATMOS FORLI-v20151001 output netcdf files (available from 20071001 to 20200226) and the variables contained in the EUMETSAT FORLI-v20151001 ozone profile output netcdf files (from 4 December 2019), respectively.

Table 3.10a: Variables in the NetCDF files provided from 20071001 to 20200226. N_{alt} denotes the number of vertical layers, N_{obs} denotes number of IASI observations included in each daily netcdf file and N_{pres} the number of pressure levels used to define inversion layers.

Parameter	Unit	Dimension	Description
latitude	degrees	$1 \times N_{obs}$	latitude of the ground pixel
longitude	degrees	$1 \times N_{obs}$	longitude of the ground pixel
Time	HHMMSS	$1 \times N_{obs}$	hour in the day as hhmmss
sun_zen_angle	degrees	$1 \times N_{obs}$	solar zenith angle at the Earth's surface for the pixel center
satellite_zen_angle	degrees	$1 \times N_{obs}$	MetOp zenith angle at the Earth's surface for the pixel center
orbit_number	-	$1 \times N_{obs}$	MetOp orbit number
scanline_number	-	$1 \times N_{obs}$	scanline number in the MetOp orbit
pixel_number	-	$1 \times N_{obs}$	pixel number in the current scanline
cloud_cover	%	$1 \times N_{obs}$	EUMETSAT Cloud coverage in the pixel
DOFS	-	$1 \times N_{obs}$	degrees of freedom of the signal in the retrieved ozone partial column profile
retrieval_quality_flag	-	$N_{alt} \times N_{obs}$	retrieval quality flag summarizing processing flags
surface_altitude	m	$1 \times N_{obs}$	altitude of the surface
tropopause_altitude	m	$1 \times N_{obs}$	tropopause altitude (from Eumetsat IASI L2 atmospheric profile with WMO definition)

thermal_contrast	K	$1 \times N_{obs}$	thermal contrast (defined as difference between Eumetsat skin temperature and Eumetsat atmospheric temperature at the first level, just above the surface)
ozone_total_column	$mol.m^{-2}$	$1 \times N_{obs}$	total column ozone
ozone_partial_column_profile	$mol.m^{-2}$	$N_{alt} \times N_{obs}$	Ozone partial column vertical profile
ozone_partial_column_error	$mol.m^{-2}$	$N_{alt} \times N_{obs}$	Vertical profile of total retrieved error
ozone_apriori_partial_column _profile	$mol.m^{-2}$	$N_{alt} \times N_{obs}$	Ozone a priori partial columns vertical profile
air_partial_column_profile	$mol.m^{-2}$	$N_{alt} \times N_{obs}$	air partial column vertical profile in the layers defined by the levels given in the variable atmosphere_pressure_grid
atmosphere_pressure_grid	hPa	$N_{pres} \times N_{obs}$	pressures 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_kernels_matrix	DU/DU	$N_{alt} \times N_{alt} \times N_{obs}$	ozone partial column averaging kernels matrix (DU/DU) in the layers defined by the levels given in the variable atmosphere_pressure_grid

Table 3.10b: Variables contained in the profile netcdf files provided from 20191204. N_{alt} denotes the number of vertical layers, N_{obs} denotes number of IASI observations included in each daily netcdf file and N_{pres} the number of pressure levels used to define inversion layers.

Parameter	Unit	Dimension	Description
time	Second	$1 \times N_{obs}$	UTC observation time in seconds since 2007-01-01 00:00:00 UTC
time_string		$1 \times N_{obs}$	UTC observation time as YYYYMMDDThhmmssZ
time_in_day	Second	$1 \times N_{obs}$	UTC observation time in seconds in the day
latitude	degrees_north	$1 \times N_{obs}$	latitude of ground pixel center
longitude	degrees_east	$1 \times N_{obs}$	longitude of ground pixel center
solar_zenith_angle	Degrees	$1 \times N_{obs}$	solar zenith angle at the Earth s surface for the pixel center
satellite_zenith_angle	Degrees	$1 \times N_{obs}$	Metop zenith angle at the Earth s surface for the pixel center
orbit_number	-	$1 \times N_{obs}$	Metop orbit number
scanline_number	-	$1 \times N_{obs}$	scanline number in the Metop orbit
pixel_number	-	$1 \times N_{obs}$	pixel number in the current scanline
ifov_number	-	$1 \times N_{obs}$	field of view number in the 2 x 2 observation matrix

retrieval_quality_flag	-	$1 \times N_{obs}$	retrieval quality flag summarizing processing flags
surface_altitude	m	$1 \times N_{obs}$	altitude of the surface
tropopause_altitude	m	$1 \times N_{obs}$	altitude of the tropopause (from Eumetsat IASI L2 atmospheric profile with WMO definition)
O3_apriori_partial_column_profile	$mol.m^{-2}$	$N_{obs} \times N_{alt}$	ozone a priori partial column vertical profile retrieved in the layers defined by the levels given in the variable atmosphere_pressure_grid
O3_partial_column_profile	$mol.m^{-2}$	$N_{obs} \times N_{alt}$	ozone partial column vertical profile retrieved in the layers defined by the levels given in the variable atmosphere_pressure_grid
O3_partial_column_error	$mol.m^{-2}$	$N_{obs} \times N_{alt}$	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
air_partial_column_profile	$mol.m^{-2}$	$N_{obs} \times N_{alt}$	air partial column vertical profile in the layers defined by the levels given in the variable atmosphere_pressure_grid
atmosphere_pressure_grid	Pa	$N_{obs} \times N_{pres}$	pressures 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	$(mol.m^{-2})/(mol.m^{-2})$	$N_{obs} \times N_{alt} \times N_{alt}$	ozone partial column averaging kernels matrix in the layers defined by the levels given in the variable atmosphere_pressure_grid
O3_total_degrees_of_freedom	-	$1 \times N_{obs}$	degrees of freedom of the signal in the retrieved ozone partial column profile

3.7. L3 Nadir Merged Ozone Profiles (GOP-ECV) (DLR)

Note that the first version of this product has not yet been generated.

3.7.1. Input data and algorithm

3.7.2. Parameters

3.8. L2 HARMonized Limb Ozone Profiles (HARMOZ) (Bremen)

3.8.1. Input data and algorithm

Table 3.11: List of the datasets used in HARMOZ

Instrument	L2 data version	Last HARMOZ version

GOMOS	v6	fv0004
SCIAMACHY	v3.5	fv0004
MIPAS	v221	fv0004
OSIRIS	v5.7	fv0007
SMR	v3.1	fv0003
ACE-FTS	v3.5/3.6	fv0002
MLS	v4.2	fv0007 (using ERA5)
OMPS-LP (Usask)	v1.0.2	fv0002
POAM III	v4	fv0001 (no quality flags), fv0002
SAGE III ISS	v2	fv0002 (using ERA5)
SAGE III Meteor 3M	v4	fv0002 (using ERA5)
SABER	v5.1	fv0005 (using ERA5)

3.8.2. Parameters

Each file contains the mandatory parameters, which are the same for all instruments (Table 3.12). The files contain also optional instrument-specific parameters (Table 3.13), which might be related to the data quality.

Table 3.12: Mandatory parameters in the HARMOZ NetCDF files. N_{alt} and N_{prof} denote the number of pressure levels and the number of profiles, respectively.

Parameter	Unit	Dimension	Description
Time	days since 1900-01-01 00:00:00	$N_{prof} \times 1$	The parameter to index the profiles
air_pressure	hPa	$N_{alt} \times 1$	The vertical coordinate
altitude	km	$N_{alt} \times N_{prof}$	The geometric altitude above the mean sea-level
latitude	degree_north	$N_{prof} \times 1$	Latitude of each profile
longitude	degree_east	$N_{prof} \times 1$	Longitude of each profile
mole_concentration_of_ozone_in_air	$mol.cm^{-3}$	$N_{alt} \times N_{prof}$	Vertical profiles of ozone. Number density (cm-3) is acquired by multiplying the variable with Avogadro constant NA=6.02214e23 mol-1
mole_concentration_of_ozone_in_air standard_error	$mol.cm^{-3}$	$N_{alt} \times N_{prof}$	Uncertainty (random error) associated with the ozone profiles
vertical_resolution	km	$N_{alt} \times N_{prof}$ or $N_{alt} \times 1$	FWHM of the averaging kernel
air_temperature	K	$N_{alt} \times N_{prof}$	Temperature profiles at the locations of measurements, for conversion from concentration to mixing ratio

Table 3.13: Optional parameters in HARMOZ NetCDF files N_{alt} and N_{prof} denote the number of pressure levels and the number of profiles, respectively.

	Parameter	Unit	Dimension	Description
GOMOS	orbit_number	-	$N_{prof} \times 1$	Envisat orbit number
	star_number	-	$N_{prof} \times 1$	Star number in GOMOS catalogue

	star_magnitude	-	$N_{prof} \times 1$	Star visual magnitude
	star_temperature	K	$N_{prof} \times 1$	Star effective temperature
	obliquity	degree	$N_{prof} \times 1$	Obliquity of occultation: the angle between the orbital plane and the line of sight
	sza	degree	$N_{prof} \times 1$	solar zenith angle at tangent point
	Chi2	-	$N_{alt} \times N_{prof}$	Profiles of normalized χ^2-statistics. Usually close to 1. Large values indicate problems with retrievals
	illumination_condition_flag	-	$N_{prof} \times 1$	0-full dark, 3-straylight, 2- twilight, 4-straylight & twilight.
	SAA_flag	-	$N_{prof} \times 1$	The indicator showing that the data might be affected by the Southern Atlantic Anomaly (cosmic rays); 0- no, 1- yes
SCIAMACHY	orbit_number	-	$N_{prof} \times 1$	Envisat orbit number
	state_id	-	$N_{prof} \times 1$	State ID of the SCIA measurement
	height_sat	km	$N_{prof} \times 1$	Satellite altitude above the sea-level, for each profile
	radius_earth	km	$N_{prof} \times 1$	The Earth radius at locations above the tangent points
	sza_tanpnt	degree	$N_{prof} \times 1$	solar zenith angle at tangent point
	pixel_lat	degree_north	$N_{prof} \times 4$	the ground latitudes of the four corners of the limb scan pixel
	pixel_lon	degree	$N_{prof} \times 4$	the ground longitude of the four corners of the limb scan pixel
	total_ozone_column	mm	$N_{prof} \times 1$	Total ozone column for each profile; 1mm=100 DU (Dobson Unit)
	systematic_error	%	$N_{alt} \times N_{prof}$	Systematic errors derived from parameter deviation simulation (see ozone-CCI ATBD)
MIPAS	apriori_temperature	K	$N_{alt} \times N_{prof}$	temperature profiles at locations of measurements based on ECMWF and MSIS data
	geo_id	-	$N_{prof} \times 22$	MIPAS geolocation identifier formatted as XXXXX_YYYYMMDDThhmmssZ where XXXXX=orbit, YYYY=year, MM=month, DD=day, hh=hour, mm=minute, ss=second
	orbit_number	-	$N_{prof} \times 1$	Envisat orbit number
	Sza	degree	$N_{prof} \times 1$	Solar zenith angle
	chi2	-	$N_{prof} \times 1$	Normalized χ^2- value of retrievals
	Dof	-	$N_{prof} \times 1$	degrees of freedom of target retrieval
	rms	$nW.cm^{-1}.sr^{-1}$	$N_{prof} \times 1$	root mean square of residual spectra
OSIRIS	scan_number		$N_{prof} \times 1$	OSIRIS scan number
	albedo		$N_{prof} \times 1$	Retrieved albedo
	ssa	degree	$N_{prof} \times 1$	Solar scattering angle
	Sza	degree	$N_{prof} \times 1$	Solar zenith angle
	optics_temperature	K	$N_{prof} \times 1$	Average optics box temperature

SMR	quality	-	$N_{prof} \times 1$	Quality flag 0: best quality, 4: tolerable
	solar_zenith_angle	degree	$N_{prof} \times 1$	
	local_solar_time	h	$N_{prof} \times 1$	
	measurement_response	-	$N_{prof} \times 1$	Proportion of measurement; measurements with weak influence of a priori have measurement response close to 1.
	scaled_potential_ vorticity	$K.m^2.kg^{-1}.s^{-1}$	$N_{alt} \times N_{prof}$	Profiles of potential vorticity (Lait, 1994) scaled at 475 K potential temperature level
	equivalent_latitude	degree	$N_{alt} \times N_{prof}$	Profiles of equivalent
ACE-FTS	beta_angle	degree	$N_{alt} \times N_{prof}$	β-angle is defined as the angle between the orbit plane of ACE-FTS and the vector
MLS	solar_zenith_angle	degree	$N_{prof} \times 1$	
	local_solar_time	h	$N_{prof} \times 1$	
	stratospheric_ozone_ column	$mol.cm^{-2}$	$N_{prof} \times 1$	stratospheric ozone column between 200 hPa and 1 hPa in mole concentration or number of moles per unit area (molarity) of ozone
	tropopause_altitude	km	$N_{prof} \times 1$	tropopause altitude derived from the thermal lapse rate WMO definition
POAM III	event_number	-	$N_{prof} \times 1$	orbit number
	hemisphere	-	$N_{prof} \times 1$	1 corresponds to Northern Hemisphere, -1 corresponds to Southern Hemisphere
	stratospheric_ozone_ column	$mol.cm^{-2}$	$N_{prof} \times 1$	stratospheric ozone column between 200 hPa and 1 hPa in mole concentration or number of moles per unit area (molarity) of ozone
	tropopause_altitude	km	$N_{prof} \times 1$	tropopause altitude derived from the thermal lapse rate WMO definition
SABER	orbit_number	-	$N_{prof} \times 1$	orbit number
	systematic_error	%	$N_{alt} \times N_{prof}$	systematic error of ozone in mole concentration or number of moles per unit volume (molarity) for SABER 2.0 ozone profiles taken from Rong et al. 2009
	solar_zenith_angle	degree	$N_{prof} \times 1$	
	stratospheric_ozone_ column	$mol.cm^{-2}$	$N_{prof} \times 1$	stratospheric ozone column between 200 hPa and 1 hPa in mole concentration or number of moles per unit area (molarity) of ozone
	tropopause_altitude	km	$N_{prof} \times 1$	tropopause altitude derived from the thermal lapse rate WMO definition
SAGE	event_number	-	$N_{prof} \times 1$	Number of the event/observation

	solar_event	-	$N_{prof} \times 1$	1 corresponds to sunrise, 2 corresponds to sunset
	stratospheric_ozone_colum	$mol.cm^{-2}$	$N_{prof} \times 1$	stratospheric ozone column between 200 hPa and 1 hPa in mole concentration or number of moles per unit area (molarity) of ozone
	tropopause_altitude	km	$N_{prof} \times 1$	tropopause altitude derived from the thermal lapse rate WMO definition
SAGE III M-3M	event_number	-	$N_{prof} \times 1$	Number of the event/observation
	solar_event	-	$N_{prof} \times 1$	1 corresponds to sunrise, 2 corresponds to sunset
	stratospheric_ozone_column	$mol.cm^{-2}$	$N_{prof} \times 1$	stratospheric ozone column between 200 hPa and 1 hPa in mole concentration or number of moles per unit area (molarity) of ozone
	tropopause_altitude	km	$N_{prof} \times 1$	tropopause altitude derived from the thermal lapse rate WMO definition

3.9. L2 OMPS-Limb Ozone Profiles (USask)

The USask OMPS-LP L2 2D Ozone v1.1 product provides ozone profile retrievals performed at the University of Saskatchewan for the central slit of the OMPS-LP instrument on the Suomi-NPP satellite. The two-dimensional retrieval algorithm accounts for variation in the along orbital track dimension, retrieving an entire orbit simultaneously instead of treating each image independently. Ozone is retrieved from the thermal tropopause to 59 km on a 1 km grid and with a vertical resolution of approximately 2 km.

Each granule contains data from the daylight portion of each orbit measured for a full month. 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 125 km.

3.9.1. Input data and algorithm

OMPS-LP L1G v2.5 are processed using the two-dimensional retrieval algorithm developed at the University of Saskatchwan.

3.9.2. Parameters

Table 3.14: List of variables in the NetCDF files

Parameter	Unit	Dimensions	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

latitude	degree_north	$N_{prof} \times 1$	Latitude of each profile
longitude	degree_east	$N_{prof} \times 1$	Longitude of each profile
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	$N_{alt} \times 1$	Averaged vertical resolution
temperature	K	$N_{alt} \times N_{prof}$	Temperature profiles at the locations of measurements from MERRA
tropopause_altitude	km	$N_{prof} \times 1$	Tropopause altitude in the OMPS-LP L1-ANC file interpolated to the retrieval grid, taken from MERRA

3.10. L3 SAGE-CCI-OMPS Limb Ozone Profiles (FMI)

3.10.1. Input data and algorithm

The merged monthly zonal mean dataset of ozone profiles, which is also referred to as the SAGE-CCI-OMPS dataset, is created using the data from several satellite instruments: SAGE II on ERBS, GOMOS, SCIAMACHY and MIPAS on Envisat, OSIRIS on Odin, ACE-FTS on SCISAT, and OMPS on Suomi-NPP. The merged dataset is created with the aim of analyzing stratospheric ozone trends. For the merged dataset, we used the latest versions of the original ozone datasets. The long-term SAGE-CCI-OMPS dataset is created by computation and merging of deseasonalized anomalies from individual instruments. The detailed description of the dataset can be found in [*Sofieva et al.*, 2017].

The merged SAGE-CCI-OMPS dataset consists of deseasonalized anomalies of ozone in 10° latitude bands from 90°S to 90°N and from 10 to 50 km in steps of 1 km covering the period from October 1984 to July 2016. For trend analyses, it is recommended using the deseasonalized anomalies. According to the merging principle, the best quality of the merged dataset is in the stratosphere below 60° latitude. For the purpose of other applications (e.g., comparisons with models), we presented also merged ozone concentration profiles. The details of computing merged number density profiles from the merged deseasonalized anomalies are presented in [*Sofieva et al.*, 2017].

3.10.2. Parameters

All data are included into one netcdf4 file, its main parameters are collected in Table 5.

Table 3.15: The variables of the SAGE-CCI-OMPS netCDF file. N_{date}, N_{alt}, N_{lat} are number of months, altitude levels and latitude zones, respectively.

	Parameter	**Unit**	**Dimension**	**Description**
General parameters	time	days since 1900-01-01	$N_{date}\times1$	one data point for each month: on the 1st of the month
	altitude	km	$N_{alt}\times1$	geometric altitude
	latitude_centers	degrees_north	$N_{lat}\times1$	Centers of latitude bins: -85°: 10°:85°
	Instruments	-	$N_{instru}\times1$	A dimension for individual datasets, instrument order: 1-GOMOS, 2-MIPAS, 3-SCIAMACHY, 4-OSIRIS, 5-ACE-FTS , 6-OMPS, 7-SAGEII
Merged data	merged_ozone_anomaly	%	$N_{date}\times N_{alt}\times N_{lat}$	Merged deseasonalized anomalies, see [Sofieva et al., 2017] for details
	merged_ozone_concentration	$mol.m^{-3}$	$N_{date}\times N_{alt}\times N_{lat}$	Vertical profiles of merged monthly zonal mean ozone mole concentration.
	uncertainty_of_merged_ozone	%	$N_{date}\times N_{alt}\times N_{lat}$	Uncertainty of the merged data
	Pressure	hPa	$N_{date}\times N_{alt}\times N_{lat}$	Mean pressure corresponding to spatiotemporal bins
	Temperature	K	$N_{date}\times N_{alt}\times N_{lat}$	Mean temperature corresponding to spatiotemporal bins
Individual datasets	ozone_anomaly_instrument	%	$N_{date}\times N_{alt}\times N_{lat}\times N_{instru}$	Deseasonalized anomalies of ozone from individual instruments
	Uncertainty_of_ozone_anomaly_instrument	%	$N_{date}\times N_{alt}\times N_{lat}\times N_{instru}$	Uncertainty of deseasonalized anomalies individual datasets

3.11. L3 Gridded Merged Limb Ozone Profiles (MEGRIDOP, FMI)

3.11.1. Input data and algorithm

The MErged GRIdded Dataset of Ozone Profiles (MEGRIDOP) in the stratosphere with a resolved longitudinal structure is derived from data by six limb and occultation satellite instruments: GOMOS, SCIAMACHY and MIPAS on Envisat, OSIRIS on Odin, OMPS on Suomi-NPP, and MLS on Aura. The merged dataset was generated as a contribution to the European Space Agency Climate Change Initiative Ozone project (Ozone_cci). The period of this merged time series of ozone profiles is from late 2001 until the end of 20, and it will be regularly extended in the future.

For the merged dataset, we used the latest versions of the original ozone datasets (Table 1). The monthly mean gridded ozone profile dataset is provided in the altitude range from 10 to 50 km in bins of 10° latitude x 20° longitude. The merging is performed using deseasonalized anomalies. The detailed description of the merging method can be found in (Sofieva et al., 2021).

Table 3.16: General information about the datasets.

Instrument/ satellite	**Level 2 processor, references**	**Years**	**Vertical range/retrieval coordinate**	**Local time of Level 2 data**
MIPAS/Envisat	KIT/IAA V7R_O3_240	2005-2012	6-70 km, Altitude	10 a.m. and p.m.

Instrument/ satellite	Level 2 processor, references	Years	Vertical range/retrieval coordinate	Local time of Level 2 data
SCIAMACHY/Envisat	UBr v3.5	2002-2012	8-65 km, Altitude	10 a.m.
GOMOS/Envisat	ALGOM2s v1	2002-2011	10-105 km, altitude	10 p.m.
OSIRIS/Odin	USask v5.10	2001-present	10-59 km, altitude	6 a.m. and p.m
OMLS-LP /SUOMI-NPP	USask 2D v 1.1.0	2012-present	6- 59 km, altitude	1:30 p.m
MLS/Aura	NASA v4.2	2004 - present	261-0.02 hPa (~8-75 km), pressure	1:30 a.m. and p.m.

3.11.2. Parameters

The merged monthly mean data with resolved longitudinal structure are collected into one NetCDF-4 file. The altitude range for LP-MERGED dataset is 10 -50 km, the data are averaged in 10° x 20° latitude-longitude bins. The variables included into NetCDF files are collected in Table 3.7.

Table 3.17: The variables in LatLon_MERGED NetCDF file. Ndate, Nalt, Nlat , Nlon are number of months, altitude levels, latitude and longitude zones, respectively.

	Parameter	Unit	Dimensions	Description
General parameters	time	days since 1984-01-01	$N_{date}\times 1$	one data point for each month: on the 1st of the month
	altitude	km	$N_{alt}\times 1$	Geometric altitude
	latitude_centers	degrees_north	$N_{lat}\times 1$	Centers of latitude bins: -85°: 10°:85°
	longitude_centers	degree_east	$N_{lon}\times 1$	Centers of longitude bins: -170°:20°:170°
	Instruments	-	$N_{instru}\times 1$	A dimension for individual datasets, instrument order 1-GOMOS, 2-MIPAS, 3-SCIAMACHY, 4-OSIRIS, 5- MLS, 6-OMPS
Merged data	merged_ozone_anomaly	%	$N_{date}\times N_{alt}\times N_{lat}\times N_{lon}$	Merged deseasonalized anomalies, see (Sofieva et al., 2020) for details
	merged_ozone_concentration	mol.m^{-3}	$N_{date}\times N_{alt}\times N_{lat}\times N_{lon}$	Vertical profiles of merged monthly zonal mean ozone mole concentration.
	uncertainty_of_merged_ozone	%	$N_{date}\times N_{alt}\times N_{lat}\times N_{lon}$	Uncertainty of the merged data
	Pressure	hPa	$N_{date}\times N_{alt}\times N_{lat}\times N_{lon}$	Mean pressure corresponding to bins
	temperature	K	$N_{date}\times N_{alt}\times N_{lat}\times N_{lon}$	Mean temperature corresponding to bins
Individual	ozone_concentration_instrument	mol.m^{-3}	$N_{date}\times N_{alt}\times N_{lat}\times N_{lon}\times N_{instru}$	Gridded ozone profiles for individual instruments
	uncertainty_of_ozone_concentration_instrument	%	$N_{date}\times N_{alt}\times N_{lat}\times N_{lon}\times N_{instru}$	Random uncertainties of the gridded ozone profiles for individual instruments

	Parameter	Unit	Dimensions	Description
	ozone_anomaly_instrument	%	$N_{date} \times N_{alt} \times N_{lat} \times N_{lon} \times N_{instru}$	Deseasonalized anomalies of ozone from individual instruments
	uncertainty_of_ozone_anomaly_instrument	%	$N_{date} \times N_{alt} \times N_{lat} \times N_{lon}$ N_{instru}	Uncertainty of deseasonalized anomalies from individual datasets

4. Using the data

4.1. *L2 Total Ozone (BIRA-IASB)*

4.1.1. Data access and format

The level-2 data sets are distributed via Net-CDF files (one file per orbit). An example of filename for the L2 total ozone column output file of one GOME orbit is:
ESACCI-OZONE-L2P-TC-GOME_ERS2-BIRA_010185-19970401143000-fv0300.nc
where:

- "GOME_ERS2" indicates the instrument and platform. Alternatively, it can be "SCIAMACHY_ENVISAT", "GOME2_METOPA", "GOME2_METOPB" , "GOME2_METOPC", "OMI_AURA" or "OMPS_Suomi-NPP".
- "010185" represents the orbit number
- "19970401143000" indicates the date and time of the beginning of the orbit. This is to be interpreted as YYYMMDDhhmmss.
- "fv0300" is the product number. This is to be interpreted as v03.00. This number may vary from a sensor to another.

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

1. Example of python3 code to read total ozone columns from one OMI L2 file and plot them as a function of pixel latitude center after masking of non-converged pixels.

```
import numpy as np
import matplotlib.pyplot as plt
from netCDF4 import Dataset

CCI_filename="ESACCI-OZONE-L2P-TC-OMI_AURA-BIRA_011767-20061001071800-fv0300.nc"
with Dataset(CCI_filename,'r') as fid:
        o3=np.array(fid.variables['total_ozone_column'])
        lat= np.array(fid.variables['latitude'])
        conv=np.array(fid.variables['convergence_flag'])
o3[conv==0]=np.nan

plt.plot(lat.ravel(),o3.ravel(),".")
plt.grid(True)
plt.xlabel("Latitude pixel center")
plt.ylabel("CCI total ozone column (mol.m-2)")
```

```
plt.title("OMI orbit #11767")
plt.show()
```

2. Example of matlab code to read total ozone columns from one OMI L2 file and plot them as a function of pixel latitude center after masking of non-converged pixels.

```
CCI_filename="ESACCI-OZONE-L2P-TC-OMI_AURA-BIRA_011767-
20061001071800-fv0300.nc";

o3=ncread(CCI_filename,'total_ozone_column');
lat=ncread(CCI_filename,'latitude');
conv=ncread(CCI_filename,'convergence_flag');
o3(conv==0)=NaN;

plot(lat(:),o3(:),'.')
grid on
xlabel("Latitude pixel center")
ylabel("CCI total ozone column (mol.m-2)")
title("OMI orbit #11767")
```

4.1.3. Preliminary evaluation

The CCI L2 total ozone datasets have been extensively validated by performing inter-satellite comparisons on one hand and comparisons with independent ground-based instruments (Brewer, Dobson and SAOZ) on the other. Results of those comparisons are extensively discussed in Koukouli et al. (2015), Chiou et al., 2014, Garane et al. (2018, 2019).

In summary, those studies has shown that the inter-sensor consistency of the individual level-2 data sets has very small mean differences (generally less than 0.5% at moderate latitudes. Compared to ground-based instruments, the mean bias between GODFIT v4 satellite ozone columns and ground data is well within 1.0±1.0% for all sensors, the drift per decade spans between −0.5% and 1.0±1.0% depending on the sensor. The quality of those data sets makes them suitable and useful for long-term analysis of the ozone layer, such as decadal trend studies, the evaluation of model simulations and data assimilation applications.

4.1.4. Contacts

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4.2. L3 Total Ozone (DLR)

4.2.1. Data access and format

The individual L3 total ozone data are provided as netCDF files (one file per month). The content of the netCDF files is listed in Table 3.4. The structure of the filenames is as follows:

ESACCI-OZONE-L3S-TC-INST-PLAT-CCI-DLR_1M-YYYYMM01-fvxxxx.nc.

INST is the shortname of the sensor (GOME, SCIA, OMI, GOME2A, or GOME2B), PLAT is the name of the platform (ERS2, ENVISAT, AURA, or METOP), YYYY denotes the year, MM the month, and xxxx is the fileversion.

4.2.2. 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 3.4.

4.2.3. Preliminary evaluation

4.2.4. Contacts

- Diego Loyola: Diego.Loyola@dlr.de

4.3. L3 Merged Total Ozone (GTO-ECV) (DLR)

4.3.1. Data access and format

The L3 merged total ozone product GTO-ECV is provided as netCDF files (one file per month). The content of the netCDF files is listed in Table 3.5. The structure of the filenames is as follows: ESACCI-OZONE-L3-TC-MERGED-CCI-YYYYMM-fvxxxx.nc. YYYY denotes the year, MM is the month, and xxxx indicates the fileversion.

4.3.2. 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 3.5.

4.3.3. Preliminary evaluation

Detailed results of the geophysical validation of GTO-ECV total ozone columns can be found in Coldewey-Egbers et al. (2015) and in Garane et al. (2018).

4.3.4. Contacts

- Diego Loyola: Diego.Loyola@dlr.de

4.4. L4 Total Ozone Multi-Sensor Reanalysis (MSR) (KNMI)

4.4.1. Data access and format

The MSR data set can be downloaded in a single netcdf data file C3S_TC_MSR2.nc via the link: http://temis.nl/protocols/o3field/data/multimission/MSR-2.nc

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

In python the datafile can be read with the following basic code:

```
from netCDF4 import Dataset

filename=' C3S_TC_MSR-2.nc'
ncfile=Dataset(filename,'r',format='NETCDF4')

ozone=ncfile.variables['Average_O3_column'][:]
month=ncfile.variables['time'][:]
lat=ncfile.variables['latitude'][:]
lon=ncfile.variables['longitude'][:]

ncfile.close()
```

For IDL and Matlab no examples are currently available.

4.4.3. Preliminary evaluation

Data quality is given in the data file. A limited evaluation is given in van der A et al. (2015). More work on the evaluation still has to be done.

4.4.4. Contacts

Contact persons for the MSR-2 data are:

- Ronald van der A: ronald.van.der.a@knmi.nl
- Marc Allaart: allaart@knmi.nl

4.5. L2 Nadir BUV Ozone Profile (RAL)

4.5.1. Data access and format

RAL L2 nadir profile data are stored in NetCDF files. Climate Forecast (CF) convention standard names are provided where applicable. Folder structure indicates instrument, platform and data version and date. Filenames are in ESA CCI convention:

ESACCI-<CCI Project>-<Processing Level>-<Data Type>-<Product String> [-<Additional Segregator>]-<IndicativeDate>[<Indicative Time>]- fv<File version>.nc

With <File version> following <fvXX.yy>, XX=major, yy=minor version. Eg. Ozone level 2 Nadir Profile, from GOME-2 on Metop-A, observation on 2nd Jan 2010 from 04:24:29 to 05:05:53 version 3.0:

ESACCI-OZONE-L2P-NP-RAL_GOME2_METOPA-20100102042429_20100102060553-fv0300.nc

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

Files may be read with standard NetCDF routines.

4.5.3. Preliminary evaluation

4.5.4. Contacts

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- Barry Latter: barry.latter@stfc.ac.uk
- Group webpage: http://rsg.rl.ac.uk or via RAL Space http://ralspace.stfc.ac.uk

4.6. L2 Nadir IASI Ozone Profile (ULB)

4.6.1. Data access and format

The Level 2 ozone profile product files from the FORLI retrievals processed at ULB or at EUMETSAT are generated for CCI by LATMOS and distributed by AERIS (https://iasi.aeris-data.fr/O3) as netcdf-4 files (one file per day). The content of the netCDF files is listed in Tables 3.10a and 3.10b.

The IASI filename currently available through AERIS is as follows:

- For the ULB-LATMOS FORLI-v20151001 files (available from 20071001 to 20200226):

  IASI_FORLI_O3_metop*X_yyyymmdd_version*.nc

- For the EUMETSAT FORLI-v20151001 files (available from 20191204):

  IASI_METOPX_L2_O3_PROFILE_*yyyymmdd*_ULB-LATMOS_*version*.nc

where *X*=a, b or c, *yyyymmdd* is the date of retrieval and *version*=the product version number.

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 3.10.

4.6.3. Preliminary evaluation

The netcdf files, generated for CCI by LATMOS and distributed by AERIS, contain only measurements meeting a series of quality criteria:

a) For the ULB-LATMOS FORLI-v20151001 files (available from 20191204):

No retrieval is performed for pixels characterized by:
- total cloud cover higher than 13%
- error related to the L1C data
- no L2 data associated with L1C data
- missing T, H2O, Pskin or cloud L2 input values

In addition, all data meeting the following criteria were also filtered out:
- spectral residual biased (lower than -0.75 x 10−9 W/(cm2 sr cm−1) or higher than 1.25 x 10−9 W/(cm2 sr cm−1))
- root-mean square of the spectral residual too large (higher than 3.5 × 10−8 W/(cm2. sr.cm−1))
- partial column of O3 is negative
- the averaging kernel matrix includes strange values (generally too high)
- the procedure diverged
- the total error covariance matrix ill conditioned

It is also recommended that some additional quality control criteria are applied to the ozone product, using parameters also supplied within the netcdf file:
- ratio of the O3 partial column from ground to 6 km to the total O3 column (COL06/COLTOT) higher or equal to 0.08
- DOFS lower than 2

Note that the netcdf files contain a variable named "ret_flag" which is a general quality flag assessing the quality of the IASI O_3 product. However, this variable is currently not available. It is equal to 0 for all observations.

The dataset 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).

b) For the EUMETSAT FORLI-v20151001 files (available from 20191204):

The netcdf files contain a variable named "retrieval_quality_flag" which is a general quality flag assessing the quality of the IASI O_3 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 used for the ULB-LATMOS FORLI-v20151001 files (see above), 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

For consistency with the IASI archive and storage purpose, the netcdf files include only observations associated with retrieval_quality_flag=1.

4.6.4. Contacts

At ULB:

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4.7. L3 Nadir Merged Ozone Profiles (GPO-ECV) (DLR)

The first version of this data record has not yet been generated.

4.7.1. Data access and format

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

4.7.3. Preliminary evaluation

4.7.4. Contacts

4.8. L2 HARMonized Limb Ozone Profiles (HARMOZ) (Bremen)

4.8.1. Data access and format

HARMOZ ozone profiles are structured in folders corresponding to each instrument. Each folder contains monthly data files with self-explanatory names: ESACCI-OZONE-L2-LP-IIII_SSSS-PP_VV-YYYYMM-Z.nc, where L2=Level 2, LP= Level2, IIII= instrument, SSSS=satellite, PP=processing center, VV= processor version, YYYY= year, MM=month, Z=file version.

For example, the file ESACCI-OZONE-L2-LP-GOMOS_ENVISAT-IPF_V6-200801-fv0004.nc contains GOMOS ozone profiles for January 2008.

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

Tables of biases between pair of instruments, as well as bias uncertainties, and comparisons of overlapping time series are provided in Sofieva et al. (2013).

4.8.4. Contacts

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4.9. L2 OMPS-Limb Ozone Profiles (Bremen)

4.9.1. Data access and format

Files are available at: https://zenodo.org/record/4014195#.X4mfkpqxWV4. Example of filename:

OZONE-L2-LP-OMPS_LP_SUOMI_NPP-SASK_2D_V1_1_0-YYYYMM-fv0001.nc

where YYYY= year and MM=month.

4.9.2. Data reading examples (IDL, Matlab, Python)

Files are written in NetCDF4 format, which can be read with standard routines (e.g. h5py and xarray in Python).

4.9.3. Preliminary evaluation

A description of the retrieval algorithm and of the obtained results, together with a comparison with MLS ozone profiles can be found in Zawada et al. (2018).

4.9.4. Contacts

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4.10. L3 SAGE-CCI-OMPS Limb Ozone Profiles (FMI)

4.10.1. Data access and format

The SAGE_CCI_OMPS dataset is collected in one netcdf-4 file: ESACCI-OZONE-LP-L3-MZM_MERGED_fv0006.nc. Its size is ~50 Mb.

The dataset can be downloaded from https://climate.esa.int/en/projects/ozone/data/ and at ftp://cci_web@ftp-ae.oma.be/esacci.

4.10.2. Data reading examples (IDL, Matlab, Python)

The netcdf-4 files can be read with many software such as IDL, Matlab, Python, Panoply. The variables written in netcdf files are specified in Sect.3.10.

4.10.3. Preliminary evaluation

The dataset has been used in several scientific publications related to analyses of ozone trends, including WMO ozone assessment, BAMS State of the Climate, and the SPARC LOTUS report.

4.10.4. Contacts

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4.11. L3 Gridded Merged Limb Ozone Profiles (FMI)

The first version of this data record has not yet been generated.

4.11.1. Data access format

4.11.2. Data reading examples (IDL, Matlab, Python)

4.11.3. Preliminary evaluation

4.11.4. Contacts

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5. Acronyms, abbreviations and definition

Acronym	Definition
ACE-FTS	Atmospheric Chemistry Experiment – Fourier Transform Spectrometer
ATBD	Algorithm Theoretical Basis Document
BIRA-IASB	Belgian royal Institute for Space Aeronomy
CCI	Climate Change Initiative
CDR	Climate Data Record
CF	Climate Forecast (Conventions and Metadata)
CNES	Centre National d'Études Spatiales (France)
CNR	Consiglio Nazionale delle Ricerche (Italy)
CRG	Climate Research Group
DARD	Data Access Requirements Document
DEM	Digital Elevation Model
DHF	Data Host Facility
DIAL	Differential Absorption Lidar
DLR	German Aerospace Centre
DOAS	Differential optical absorption spectroscopy
DoD	Department of Defense (USA)
DU	Dobson unit
ECMWF	European Centre for Medium-Range Weather Forecasts

Acronym	Definition
ECV	Essential Climate Variable
Envisat	Environmental Satellite (ESA)
EO	Earth Observation
EOF	Empirical orthogonal function
EOS	Earth Observing System
EP	Earth Probe
ERBS	Earth Radiation Budget Satellite
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
FOR	Field Of Regard
FORLI	Fast Optimal/Operational Retrieval on Layers for IASI
GAW	Global Atmosphere Watch
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)
GOMOS	Global Ozone Monitoring by Occultation of Stars
GTO	GOME-type Total Ozone
HALOE	Halogen Occultation Experiment
IAMAP	International Association of Meteorology and Atmospheric Physics
IASI	Infrared Atmospheric Sounding Interferometer
IFAC	Istituto di Fisica Applicata "Nello Carrara"
IO3C	International Ozone Commission
IPA	Independent pixel approximation
IR	Infra-Red
IRI	Infra-Red Imager
IUP	Institute of Environmental Physics, University of Bremen
ICDR	Intermediate Climate Data Record
KIT	Karlsruhe Institute of Technology
KMI-IRM	Royal Meteorological Institute of Belgium
KNMI	Royal Netherlands Meteorological Institute
LATMOS	Laboratoire Atmosphères et Observations Spatiales
LS	Low Stratosphere
LTE	Local thermodynamic equilibrium
LUT	Look-up table
Metop	Meteorological Operational Platform (EUMETSAT)
MIPAS	Michelson Interferometer for Passive Atmospheric Sounding
MLER	Minimum Lambertian Equivalent Reflectivity
MLS	Microwave Limb Sounder
MS	Multiple scattering

Acronym	Definition
MSR	Multi-Sensor Reanalysis
NASA	US National Aeronautics and Space Administration
NDACC	Network for the Detection of Atmospheric Composition Change
NetCDF	Network Common Data Form (data file format)
NKUA	National and Kapodistrian University of Athens
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
OSIRIS	Optical Spectrograph and InfraRed Imaging System (aboard Odin)
PCA	Principal component analysis
PSD	Product Specification Document
PUG	Product User Guide
RAL	Rutherford Appleton Laboratory
RMIB	Royal Meteorological Institute of Belgium
RMS	Root mean square
RT	Radiative transfer
SAA	Solar azimuth angle
SABER	Sounding of the Atmosphere using Broadband Emission Radiometry
SAGE	Stratospheric Aerosol and Gas Experiment
SBUV	Solar Backscatter Ultraviolet Radiometer
SCIAMACHY	Scanning Imaging Absorption Spectrometer for Atmospheric CHartographY (aboard Envisat)
SHADOZ	Southern Hemisphere Additional Ozonesondes programme
SMR	Sub-Millimetre Radiometer (aboard Odin)
SVD	Singular Value Decomposition
SZA	Solar Zenith Angle
TEC	Technical Expertise Centre of CNES
TIMED	Thermosphere Ionosphere Mesosphere Energetics Dynamics
TOA	Top of the atmosphere
TOMS	Total Ozone Mapping Spectrometer
TP	Tropopause
TPM	ESA Third Party Mission
UARS	Upper Atmosphere Research Satellite
UiB	Universität Bremen
UNEP	United Nations Environment Programme
UPMC	Université Pierre et Marie Curie
UT	Upper Troposphere
UV	Ultraviolet
UV-Vis	Ultraviolet and visible light
VZA	Viewing Zenith Angle
WMO	World Meteorological Organization
WOUDC	World Ozone and Ultraviolet Radiation Data Centre

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