Ozone_cci+

Product Specification Document (PSD)

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DOCUMENT CHANGE RECORD

Issue	Revision	Date	Modified items
0	4	08/04/2011	Draft version submitted to CMUG and ESA for comments
1	0	12/04/2011	- requirement tables removed, and text generally reorganised to avoid any duplication with the URD. The PSD now includes (1) a brief description of the model tools specific to the project, (2) a definition of the ozone_cci products and of their usefulness for climate-related studies, and (3) a detailed specification of the data products - data product specification tables added for columns, nadir profiles and limb profiles - cross-reference to URD tables given as appropriate
1	1	29/04/2011	Final version approved by ESA
2	0	29/06/2011	Revised version according to preliminary remarks from CMUG
2	1	01/07/2011	Time period specifications clarified and added to Table 1
3	0	15/12/2011	Following changes have been introduced, in response to remarks and suggestions from CMUG: - simplified introduction - revised product overview section ➔ includes time lines for data products to be generated in both phases of the CCI - revised product specification sections ➔ includes new introductory parts, new tables summarizing target systematic and random uncertainties for the data products, simplified product specification tables; data format specification for both level-2 and level-3 data where relevant
3	1	04/04/2012	Change accuracy/precision by systematic/random uncertainties
4	0	28/07/2014	Starting point for Ozone_cci phase 2
4	2	15/08/2014	Updates included from Chalmers, Univ. Toronto, FMI, KNMI, RAL, ULB, BIRA-IASB
4	3	22/09/2014	Updates of Table 1 and section 6.
4	4	02/10/2014	Update of IASI format Table in section 6.
4	5	02/10/2014	Minor updates in total ozone specifications
4	6	03/11/2015	Updates from BIRA-IASB, ULB and KNMI Including of tropospheric ozone products
5	0	04/12/2017	Final version with many revisions from all partners involved.
6	0	05/03/2024	Starting point for Ozone_cci+ phase 2
6	1	19/01/2025	Draft version submitted to ESA for comments
6	2	17/03/2025	Document header, approved by ESA
7	0	11/06/2025	Starting point for Ozone cci+ phase 3: - Inclusion of products to be developed in Phase3

			- Removal of Phase 2 products which are not to be further developed in Phase 3
7	1	28/11/2025	Inclusion of GEO requirements

Executive Summary

This Product Specification Document (PSD) defines the precise content of the total column, tropospheric column, nadir profile and limb profile ozone products to be delivered in the third phase of the Ozone_cci+ project (2025-2026). Information in this PSD will be transferred to the Product User Guide (PUG) when the ozone products are made available to the users.

Product specifications for other and/or older ozone products generated during earlier phases of the project can be found at https://climate.esa.int/en/projects/ozone/key-documents.

This PSD document

- specifies the planned content of the ozone data products to be delivered to the users, including:
  - geophysical variables and their associated uncertainties;
  - definition of the variable names and their meanings;
  - resolution and spatio-temporal sampling and coverage;
  - ancillary outputs;
  - precise specification of the format, metadata content, and digital encoding;
  - unique product and processor version identification;
- includes a list of all input data per product;
- includes estimates of the total data volume of all generated data sets.

Table of Contents

1 Introduction

1.1 Purpose

This Product Specification Document (PSD) contains detailed specifications for the Climate Data Records (CDR) developed within and produced by ESA's Ozone_cci+ project for the Essential Climate Variable (ECV) Ozone. It builds on the User Requirement Document (URD v4.0) established by the project's Climate Research Group (CRG) and on general specifications for CCI ECV products (CCI Data Standards v2.3, [AD-3]).

Overall, the aim of ESA's Climate Change Initiative is to develop ECV products that meet the needs of the Global Climate Observing System (GCOS-244 [RD-1], GCOS-245 [RD-2]). Although algorithm developments and data characterisation work to be performed in Ozone_cci+ will lead to significant progress towards meeting the climate user requirements, it must be noted that mature data products do not necessarily exist yet. The purpose of the present document is to outline the current product specifications for each ozone data product with the understanding that this specification may be incomplete and/or is expected to change in the course of the project.

1.2 Applicable documents

[AD-1] CCI+ SOW: ESA Climate Change Initiative Extension (CCI+) Phase 2: New R&D on CCI ECVs – Statement of Work, Ref. ESA-EOP-SC-AMT-2021-46, Issue 1 Revision 0, 14/02/2022.

[AD-2] CCI+ Ozone Technical Proposal: ESA Ozone_cci+ Technical Proposal – Essential Climate Variable (ECV) - Ozone, Proposal to ESA in response to RFP CCN1 to 4000126562/19/I-NB–Ozone_cci, 20/05/2022.

[AD-3] CCI Data Standards, Ref. CCI-PRGM-EOPS-TN-13-0009, Issue 2 Revision 3, 26/07/2021. Available at https://climate.esa.int/media/documents/CCI_DataStandards_v2-3.pdf

[AD-4] CCI Data Policy, Ref. CCI-PRGM-EOPS-TN-13-0019, Issue 1 Revision 1, 12/07/2013. Available at https://climate.esa.int/media/documents/CCI_Data_Policy_v1.1.pdf

1.3 Reference documents

[RD-1] The 2022 GCOS Implementation Plan, GCOS-244, October 2022. Available at https://library.wmo.int/idurl/4/58104

[RD-2] The 2022 GCOS ECVs Requirements, GCOS-245, October 2022. Available at https://library.wmo.int/idurl/4/58111

[RD-3] URD, Ozone CCI+ User Requirements Document, Ozone_cci+_D1.1_URD_v5.1, Issue 5, Revision 1, November 2025. Available at https://climate.esa.int/en/projects/ozone/key-documents.

[RD-4] ATBD, Ozone CCI+ Algorithm Theoretical Basis Document, Ozone_cci+_D2.1_ATBD_v4.2, Issue 4, Revision 2, June 2025. Available at https://climate.esa.int/en/projects/ozone/key-documents.

[RD-5] PUG, Ozone CCI+ Product User Guide, Ozone_cci+_D4.2_PUG_v2.1, Issue 2, Revision 1, March 2025. Available at https://climate.esa.int/en/projects/ozone/key-documents.

[RD-6] PVIR, Ozone CCI+ Product Validation and Intercomparison Report, Ozone_cci+_D4.1_PVIR_v5.2, Issue 5, Revision 2, March 2025. Available at https://climate.esa.int/en/projects/ozone/key-documents.

[RD-7] Hersbach, H, Bell, B, Berrisford, P, et al. The ERA5 global reanalysis. Q J R Meteorol Soc. 2020; 146: 1999–2049. https://doi.org/10.1002/qj.3803

1.4 Acronyms

ACE-FTS	Atmospheric Chemistry Experiment – Fourier Transform Spectrometer
ADP	Algorithm Development Plan
BIRA-IASB	Royal Belgian Institute for Space Aeronomy
BUV	Backscatter Ultraviolet
C3S	Copernicus Climate Change Service
CCD	Convective Cloud Differential
CCI	Climate Change Initiative
CDR	Climate Data Record
CRG	Climate Research Group
CTM	Chemistry Transport Model
DLR	German Aerospace Centre
ECMWF	European Centre for Medium-range Weather Forecast
ECV	Essential Climate Variable
ENVISAT	Environmental Satellite (ESA)
EO	Earth Observation
ESA	European Space Agency
EU	European Union
EUMETSAT	European Organisation for the Exploitation of Meteorological Satellites
FMI	Finnish Meteorological Institute
GAW	Global Atmosphere Watch
GCOS	Global Climate Observation System
GOME	Global Ozone Monitoring Experiment
GOME-2	Global Ozone Monitoring Experiment – 2
GOMOS	Global Ozone Monitoring by Occultation of Stars

GOP	GOME-type Ozone Profile
GTO	GOME-type Total Ozone
GTTO	GOME-type Tropical Tropospheric Ozone
IASI	Infrared Atmospheric Sounding Interferometer
IR	Infrared
IUP-UB	Institute of Environmental Physics, University of Bremen
JPSS	Joint Polar Satellite System
KNMI	Royal Netherlands Meteorological Institute
MetOp	Meteorological Operational Platform (EUMETSAT)
MIPAS	Michelson Interferometer for Passive Atmospheric Sounding
MLS	Microwave Limb Sounder
MW	MicroWave
NASA	National Aeronautics and Space Administration
NDACC	Network for the Detection of Atmospheric Composition Change
OMI	Ozone Monitoring Instrument
OMPS	Ozone Mapping and Profiler Suite
OSIRIS	Optical and Spectroscopic Remote Imaging System
PSD	Product Specifications Document
RAL	Rutherford Appleton Laboratory
R&D	Research & Development
S5P	Sentinel-5 Precursor
SAGE	Stratospheric Aerosol and Gas Experiment
SBUV	Solar Backscatter Ultraviolet
SCIAMACHY	Scanning Imaging Absorption Spectrometer for Atmospheric CHartography
SILAM	System for Integrated modeLling of Atmospheric coMposition
Suomi-NPP	Suomi National Polar-orbiting Partnership
TIR	Thermal Infrared
TOMS	Total Ozone Mapping Spectrometer
TPM	Third Party Mission
TROPOMI	Tropospheric Ozone Monitoring Instrument
ULB	Université Libre de Bruxelles
URD	User Requirements Document
UV	UltraViolet

2 Overview of Ozone_cci+ products

This section summarizes the different ozone data products that will be generated and made available to users at the end of the project. Table 2.1 lists some specifications of the planned product, grouped by type : total column (TC), tropospheric column (TRC), nadir profile (NP) and limb profile (LP). Although the primary Ozone_cci+ products are multi-sensor merged data sets, i.e., level-3 and level-4 data, several intermediate level-2 data sets will be produced as input for the generation of the multi-sensor data sets. We distinguish between, respectively, level-3 or level-4 data depending on whether they result from simple spatio-temporal binning of observations only, or from model-based assimilation tools.

Detailed specifications of each data product are given in the following sections.

2.1 Tropospheric ozone

Three complementary techniques are employed by the project team to derive tropospheric ozone column data.

The *Convective Cloud Differential* (CCD) technique combines total ozone and cloud information from a nadir sensor to infer tropospheric columns in the tropical belt (20°S-20°N) since 1995. One gridded multi-sensor merged product is planned, combining data from seven GOME-type sensors (GOME, SCIAMACHY, OMI, GOME-2A, GOME-2B, GOME-2C and TROPOMI).

The *Limb-Nadir Matching* (LNM) technique allows global coverage, combining total ozone column data from nadir sensor(s) and integrated ozone profile information from limb sounders since the early/mid 2000s. In Phase 2, two gridded products were created, one of which uses the OMI nadir sensor as a source of total column data while the other uses the multi-sensor merged GTO-ECV total ozone data record developed in earlier phases of CCI. In Phase 3, GTO-LIMB dataset will be further developed.

Using *Optimal Estimation*, the vertical profile of ozone is retrieved from nadir measurements in the UV-visible or infrared region. The lowest layer in these profiles is located in the troposphere. These tropospheric columns are not released as a separate product, but can be extracted from the nadir profile data products (NP identifier).

2.2 Nadir profile

Spectral measurements by nadir sensors allow the retrieval of ozone profiles at a vertical resolution of 10-15 km [RD-6]. Several level-2 (single profiles) and level-3 (gridded in time and horizontal domain) data products are envisaged for sensors operating in the UV-visible (GOME-type sensors) and the infrared (IASI sensors) spectral ranges. These are identified by NP_L2 or NP_L3.

RAL's updated UV retrieval scheme is applied to 6 sensors (ERS-2 GOME, OMI, GOME-2A, GOME-2B, GOME-2C and TROPOMI). The resulting level-2 data products contain individual ozone profiles from surface to 80 km spanning each mission's lifetime. In this CCI phase, the version of the RAL scheme which has been developed as the operational tropospheric ozone processor for Sentinel 4 will be applied to process a test month from the geostationary UV sounders GEMS and TEMPO. These geostationary sounders (including Sentinel-4) lack observations in the Hartley band (< 300 nm), so have limited information on the stratospheric profile. Therefore, only a few sub-column amounts are reported. Currently these are as follows: Surface-421 hPa (representative of tropospheric column), 421-177 hPa and total column.

The GOP-ECV (GOME-type Ozone Profile Essential Climate Variable) data record merges RAL's level-2 profile data from seven nadir UV-visible satellite sensors (GOME, SCIAMACHY, OMI, GOME-2A and GOME-2B) in a homogeneous record. The data product represents monthly mean ozone partial columns since 1995 covering 0-80 km at 5° x 5° horizontal resolution.

The FORLI-O3 retrieval scheme is applied to the IASI sensors onboard the MetOp-A, -B and -C platforms. The resulting three level-2 data products contain individual ozone profiles from surface to 60 km from the morning and evening orbits, spanning each mission's lifetime.

The IASI level-2 data sets (IASI L2 ULB-LATMOS FORLI-v20191122; processed at ULB) are combined in a daily 1° x 1° gridded ozone profile product, starting in 2008.

2.3 Limb profile

Spectral measurements by limb and occultation sounders allow the retrieval of the vertical distribution of ozone with a resolution of 1-5 km [RD-6].

The retrieval of ozone profiles from OMPS-LP observations onboard the NOAA-21 platform is performed at IUP-UB. This L2 product extends vertically from 8.5 km (or cloud to height) to 60.5 km with a vertical sampling of 1 km. The vertical resolution is typically about 2-3 km, whereas the horizontal resolution of about 200 km along track and 3 km across track. Data are available from February 2023.

A merging of the OMPS-NPP data set with the NOAA-21 product is under development. This involves L3 monthly data from the two sensors, gridded in 5° latitude x 20 ° longitude bins, with a vertical sampling of 1 km. This merged product spans the period from 2012 to present.

In addition, we are planning to develop further the following merged limb profile datasets:

- SAGE-CCI-OMPS+
- MEGRIDOP
- LIMB-HIRES
- LIMB-UTLS

Table 2.1: Specifications of the ozone data products planned for the Ozone_cci+ Climate Research Data Package. The sampling resolution is reported here, which may differ from the actual resolution. Date sets marked in blue will be delivered to CCI via UK national funding.

Product identifier	Source / processing center	Proc-essing level	Time		Vertical		Horizontal	
			Coverage	Resolution	Coverage	Resolution	Coverage	Resolution
Tropospheric ozone								
TRC_CHORA_MERGED	IUP-UB/BIRA	L3	1995-2025	monthly	sfc - 270 hPa	n/a	20°S – 20°N	1° x 1°
TRC_GTO_LIMB	FMI	L3	2004-2025	monthly	sfc - LRT km	n/a	88°S – 88°N	1° x 1°
Nadir profile								
NP_GOME	RAL	L2	1995-2011	daily	0-80 km	4-6 km	global	320 km x 40 km
NP_GOME2A	RAL	L2	2007-2020	daily	0-80 km	4-6 km	global	160 km x 160 km
NP_GOME2B	RAL	L2	2013-2023	daily	0-80 km	4-6 km	global	160 km x 160 km
NP_GOME2C	RAL	L2	2019-2024	daily	0-80 km	4-6 km	global	160 km x 160 km
NP_OMI	RAL	L2	2004-2024	daily	0-80 km	4-6 km	global	50 km x 50 km
NP_S5P	RAL	L2	2018-2024	daily	0-80 km	4-6 km	global	15 km x 38 km
NP_GOP_ECV	DLR	L3	1995-2024	monthly	0-80 km	4-6 km	global	5° x 5°
NP_IASI_MERGED	ULB/AC SAF	L3	2008-2025	daily	0-60 km	1 km	global	1° x 1°
NP_TEMPO	RAL	L2	TBC test month	hourly	0-80km	Tropospheric, and total column amounts	North America	~10x10 km
NP_GEMS	RAL	L2	TBC test month	hourly	0-80km		South-East Asia	~10x10 km
Limb profile								
LP_OMPS_N21_IUP	IUP-UB	L2	2023-2025	daily	8.5-60.5 km	2-3 km	82°S – 82°N	200 km x 3 km
LP_OMPS_MERGED	IUP-UB	L3	2012-2025	monthly	8.5-60.5 km	2-3 km	82°S – 82°N	5° lat x 20° lon
LP_L3_HIRES	FMI	L3	2002->	daily	900-0.02 hPa	1 km	global	1° x 1°
LP_SAGE-CCI-OMPS+	FMI	L3	1984->	monthly	10-50 km	1 km	global	10°
LP_MEGRIDOP	FMI	L3	2002 ->	monthly	10-50 km	1 km	global	10° x 20°

LP_LIMB-UTLS	FMI	L3	1984 - 2024	monthly	15 km near tropopause	1 km?	global	10°

Abbreviations used: sfc=surface, TOA=top of atmosphere; LRT=lapse-rate tropopause.

3 Tropospheric ozone

Three complementary techniques are employed to derive tropospheric ozone column data products: Cloud Height and Ozone Referencing Algorithm (CHORA/CCD), Limb-Nadir Matching (LNM) and Optimal Estimation. The specifications of the three product types differ because of the different inherent capabilities of the measurement technique.

In this section, the specifications for the first two product types are expressed (CHORA and LNM). Specifications for the Optimal Estimation (i.e., ozone profile retrieval from nadir sensors) products can be found in Sect. 4, since the layer containing tropospheric ozone information can be extracted from the nadir profile products (that also cover stratosphere and upper atmosphere).

3.1 Tropical Tropospheric Ozone CHORA/CCD (Level-3)

The Convective Cloud Differential (CCD) technique combines total ozone and cloud information from a nadir sensor to compute a tropospheric column of ozone over clear-sky scenes. The CCD technique is limited to the tropical belt (20°S-20°N) and covers part of the troposphere (surface to 270/200 hPa or 10/12 km). The IUP-UB harmonization scheme (IHS-NADIR) then aggregates, adjusts and merges the CCD tropospheric columns from seven UV-visible nadir sounders. This leads to a gridded data product representing the monthly mean tropospheric ozone column over the tropics since 1995.

3.1.1 Used input data

The CCD technique relies on the availability of collocated total ozone column and cloud data. Here we use the CHORA algorithm from IUP-UB. Data from seven UV-visible nadir sensors will be considered, starting with GOME in 1995 and continuing to this day with several sensors based on an evolved GOME instrument design. For each of these sensors the same level-2 algorithm will be used to maximise consistency of the time series.

Table 3.1: TRC_CHORA_MERGED data product – list of input data sets.

Sensor	Time period	L2 version	Comment
GOME	07/1995 – 06/2003	GODFIT v4	
SCIAMACHY	08/2002 – 03/2012	GODFIT v4	
OMI	10/2004 – present	GODFIT v4	Extended by the C3S service.
GOME-2A	01/2007 – 12/2019	GODFIT v4	
GOME-2B	01/2013 – present	GODFIT v4	Extended by the C3S service.

Sensor	Time period	L2 version	Comment
GOME-2C	07/2019 – present	GODFIT v4	Extended by the C3S service.
TROPOMI	05/2018 – present	RPRO/OFFL V2.4.1/2.8.0	Extended as part of ESA's ATM-MPC. The processor uses the GODFIT v4 algorithm.

3.1.2 Resolution and coverage in space and time

Table 3.2 provides an overview of the technical specifications of the CHORA-MERGED data product. It covers the tropical belt and contains two partial columns between surface-200 hPa (~12 km) and surface-270 hPa (~10 km). In the tropics, these columns cover a bit more than half the troposphere.

Table 3.2: CHORA-MERGED data product – sampling resolution and coverage in space and time.

Dimension	Specification	Notes
Temporal resolution	monthly	
Temporal coverage	07/1995 – present	
Horizontal resolution	1° x 1°	
Horizontal coverage	20°S – 20°N, 180°W – 180°E	
Vertical resolution	n/a	
Vertical coverage	surface to 270 hPa / 200 hPa	Two partial columns are provided (270 hPa ≈ 10 km; 200 hPa ≈ 12 km).

3.1.3 Uncertainty estimates, quality indicators, and expected accuracy

The expected quality of CHORA-MERGED is summarised in Table 3.3.

Table 3.3: Expected quality of CHORA-MERGED data product.

Quantity	Specification	Notes
Accuracy : systematic component	< 25%	
Accuracy : random component	< 25%	
Stability	Tbd	Pending validation

3.1.4 Product layers, auxiliary output, format and metadata

The file format used for storing the data is NetCDF-4 classic. The NetCDF Climate and Forecast (CF) Metadata Conventions standard names are used for the main variables and global attributes, to ensure compliance with CCI Data Standards [AD-3]. Table 3.4 lists the name, units, dimensions and a description of the data variables. Table 3.5 presents the included metadata.

Table 3.4: CHORA-MERGED data product – List of variables and description.

Variable	Unit	Dimension	Longname / description / comment
latitude	degree N	N_{lat}	40 elements, between -20 and +20
longitude	degree E	N_{lon}	360 elements, between -180 and +180
tropospheric_ozone_column	mol m^{-2}	N_{lat} x N_{lon}	ozone column below the 270 / 200 hPa level, top pressure is give as attribute troposphere_mole_content_ of_ozone
tropospheric_ozone_column_ error	mol m^{-2}	N_{lat} x N_{lon}	random uncertainty
tropospheric_ozone_column_ number	n/a	N_{lat} x N_{lon}	number of measurements per grid cell
tropospheric_ozone_mixingratio	mol/mol	N_{lat} x N_{lon}	column divided by the pressure difference to the surface
tropospheric_ozone_mixingratio_ error	mol/mol	N_{lat} x N_{lon}	column_error divided by the pressure difference to the surface
stratospheric_ozone_column	mol m^{-2}	N_{lat} x N_{lon}	ozone column above top pressure
stratospheric_ozone_column_ error	mol m^{-2}	N_{lat} x N_{lon}	random uncertainty ozone column above top pressure
stratospheric_ozone_column_ number	n/a	N_{lat} x N_{lon}	number of measurements per grid cell
stratospheric_ozone_column_ reference	mol m^{-2}	N_{lat}	average stratospheric_ozone_column in the reference area
stratospheric_ozone_column_ reference_error	mol m^{-2}	N_{lat}	uncertainty stratospheric_ozone_ column in the reference area
stratospheric_ozone_column_ reference_number	n/a	N_{lat}	number of stratospheric_ozone_ column in the reference area
stratospheric_ozone_column_ reference_quality_flag	n/a	N_{lat}	quality of stratospheric columns in the reference area
total_ozone_column	mol m^{-2}	N_{lat} x N_{lon}	averaged total ozone column per grid cell (total_ozone_column - stratospheric_ozone_column _reference = tropospheric_ozone _column)
total_ozone_column_error	mol m^{-2}	N_{lat} x N_{lon}	uncertainty in total column
total_ozone_column_number	n/a	N_{lat} x N_{lon}	number of measurements per grid cell
cloud and surface data			

Table 3.5: CHORA-MERGED data product – List of metadata.

Metadata name	Comment
temporal_resolution	
processing_centre	
reference	
creator_name	
creator_email	
processing_time	
base_product	
base_product_version	
product_algorithm_Name	
product_algorithm_version	
product_format_type	
product_format_version	
product_content	
projects	
geospatial_latitude_min	
geospatial_latitude_max	
geospatial_latitude_resolution	
geospatial_latitude_units	
geospatial_longitude_min	
geospatial_longitude_max	
geospatial_longitude_resolution	
geospatial_longitude_units	
geospatial_vertical_range_bottom_troposphere	
geospatial_vertical_range_top_pressure_troposphere	
geospatial_vertical_range_bottom_pressure_stratospher e	
geospatial_vertical_range_top_stratosphere	
geospatial_vertical_range_bottom_total	
geospatial_vertical_range_top_total	
geospatial_vertical_range_units	
Instruments	
Satellites	
Source	
time_coverage_start	
time_coverage_end	
minimum_strat_ref_number	
minimum_strat_ref_column	
maximum_strat_ref_err	
maximum_strat_ref_slope	

3.1.5 Data volume

An estimate of the file sizes is given in Table 3.6.

Table 3.6: CHORA-MERGED data product– Estimates of data volume.

	Month	Year	Full period
Data volume	1.2 MB	14.4 MB	400 MB

3.2 Limb-Nadir matched Tropospheric Ozone (Level-3)

The Limb-Nadir Matching (LNM) technique combines total ozone column data from nadir sensors (GTO-ECV) and stratospheric ozone profile data from limb sensors (LIMB-HIRES, Section 5.1). The product contains two tropospheric columns: one from surface to thermal tropopause, another from surface to 3 km below the thermal tropopause.

3.2.1 Used input data

The LNM technique relies on the availability of total ozone column and limb ozone profile data. The considered limb data are described in Section 5.1.

Table 3.7: GTO-LIMB data product – list of input data sets.

Sensor / data set	Time period	Data version	Comment
GTO-ECV	1995 – present	GTO-ECV L3 v3.0	multi-sensor total ozone (L3)
High-resolution merged limb	2001 – present	(see Section 5.1)	ozone profile (L3)

3.2.2 Resolution and coverage in space and time

Table 3.8 provides an overview of the technical specifications of the GTO-LIMB data product. These provide monthly mean tropospheric ozone for two partial columns since early 2000s.

Table 3.8: GTO-LIMB data product – sampling resolution and coverage in space and time.

Dimension	Specification	Notes
Temporal resolution	monthly	
Temporal coverage	GTO-LIMB: 2002 – present	
Horizontal resolution	1° x 1°	
Horizontal coverage	global	
Vertical resolution	n/a	
Vertical coverage	surface to lapse-rate tropopause; surface to 3 km below lapse-rate tropopause	two partial columns are provided

3.2.3 Uncertainty estimates, quality indicators, and expected accuracy

The expected quality of GTO-LIMB is summarised in Table 3.9.

Table 3.9: Expected quality of GTO-LIMB data product.

Quantity	Specification	Notes
Accuracy : systematic component	tbd	Pending validation
Accuracy : random component	3-9 DU (typically ~6 DU)	
Stability	tbd	Pending validation

3.2.4 Product layers, auxiliary output, format and metadata

The file format used for storing the data is NetCDF-4 classic. The NetCDF Climate and Forecast (CF) Metadata Conventions standard names are used for the main variables and global attributes, to ensure compliance with CCI Data Standards [AD-3]. Table 3.10 lists the name, units, dimensions and a description of the data variables. Table 3.11 presents the included metadata.

Table 3.10: GTO-LIMB data product – List of variables and description.

Variable	Unit	Dimension	Longname / description / comment
time			string MM-YYYY
latitude	degree N	N_{lat}	
longitude	degree E	N_{lon}	
TrOC_belowTP	DU	N_{lat} x N_{lon}	Tropospheric ozone column from the ground to 3 km below the thermal tropopause. Conversion factor to mol m^{-2} is provided.
TrOC_belowTP_error	DU	N_{lat} x N_{lon}	Estimated random error of tropospheric ozone column from ground to 3 km below the tropopause
TrOC_fromTP	DU	N_{lat} x N_{lon}	Tropospheric ozone column from the ground to the thermal tropopause. Conversion factor to mol m^{-2} is provided.
TrOC_fromTP_error	DU	N_{lat} x N_{lon}	Estimated random error of tropospheric ozone column from ground to the tropopause
mean_tropopause_altitude	km	N_{lat} x N_{lon}	Mean tropopause height in the considered month
mean_tropopause_pressure	hPa	N_{lat} x N_{lon}	Mean tropopause pressure in the considered month

Variable	Unit	Dimension	Longname / description / comment
mean_3km_below_tropopause_pressure	hPa	N_{lat} x N_{lon}	Mean pressure of the level 3 km below the tropopause in the considered month

Table 3.11: GTO-LIMB data product – List of metadata.

Metadata name	Comment
Title	Tropospheric ozone column from combination of OMI and limb instrument ozone data
Institution	Finnish Meteorological Institute
Source	Ozone data from OMI/GTO, MLS, GOMOS, SCIAMACHY, MIPAS, OSIRIS, ACE-FTS, OMPS-LP, SAGE III/ISS
History	Original development: SUNLIT project (2020). Further development: CCI+ (2022-2026).
creator_name	
creator_email	
geospatial_lat_resolution	1 deg
geospatial_lon_resolution	2 deg
geospatial_lat_min	-88 deg
geospatial_lat_max	88 deg
geospatial_lon_min	-180 deg
geospatial_lon_max	180 deg
value_for_nodata	NaN

3.2.5 Data volume

An estimate of the file sizes is given in Table 3.12.

Table 3.12: GTO-LIMB data product – Estimates of data volume.

	Month	Year	Full period
Data volume	1.6 MB	20 MB	400 MB

4 Nadir profile

Satellite observations at nadir are the most effective way to obtain global information on the horizontal distribution of ozone, together with coarse vertically resolved information (~10-15 km). CCI+ is contributing to the development of a set of level-2 ozone profile data products retrieved from nadir measurements in the UV and TIR spectral ranges. Two level-3 profile products are being developed, one combining the GOME-type sensors, the other the IASI sensors.

4.1 UV-visible Ozone Profile (Level-2)

RAL prototype level-2 scheme will be used to process vertical profiles of ozone for four UV-visible nadir sounders.

4.1.1 Used input data

Data from four UV-visible nadir sensors are considered, starting with ERS-2 GOME in 1995 and continuing to present with several sensors based on an evolved GOME instrument design.

Table 4.1: GOME-type RAL data products – list of input data sets.

Sensor	Time period	L1 version	Comment
GOME	06/1995 – 07/2011	GDP 5.1	
GOME-2A	07/2007 – 12/2020	EUMETSAT L1 v6.3 and v7.0	
GOME-2B	01/2013 – 12/2022	EUMETSAT L1 v6.3 and v7.0	
GOME-2C	01/2019 – 12/2024	EUMETSAT L1 v6.3 and v7.0	
OMI	10/2004 – 12/2024	NASA Collection 4	Uses Collection 3 L2 cloud products
S5p	05/2018 – 12/2024	ESA reprocessed v2.01	
TEMPO	Test month TBC	SAO L1 Version 3	
GEMS	Test month TBC	Korean National Environmental Satellite Centre (NESC) L1C v1.2.4	

4.1.2 Resolution and coverage in space and time

Table 4.7 provides an overview of the technical specifications of the RAL L2 prototype data products from the polar orbiting sensors. It provides global coverage between surface and 80 km at 4-6 km sampling resolution since 2004. The effective vertical resolution of the retrievals is coarser, about 10-15 km. The resolution and coverage of the geostationary products are given in Table 2.1.

Table 4.2: GOME-type RAL data products from polar orbiting sensors – sampling resolution and coverage in space and time.

Dimension	Specification	Notes
Temporal resolution	daily	
Temporal coverage	01/1995 – 12/2024	Start time depending on sensor
Horizontal resolution	320 x 40 km (ERS-2 GOME) 160 x 160 km (GOME-2), 50 x 50 km (OMI), 15 x 38 km (S5P)	
Horizontal coverage	global	except polar night
Vertical resolution	4-6 km	effective retrieval resolution is 10-15 km
Vertical coverage	0-80 km	

4.1.3 Uncertainty estimates, quality indicators, and expected accuracy

The expected quality of RAL products is summarised in Table 4.8.

Table 4.3: Expected quality of GOME-type RAL data products.

Quantity	Specification	Notes
Accuracy : systematic component	tbd	pending validation
Accuracy : random component	tbd	pending validation
Stability	tbd	pending validation

4.1.4 Product layers, auxiliary output, format and metadata

The reprocessed scheme outputs data in a new format, almost identical to that planned for Sentinel-5 (building extensively on the operational S5P L2 format). The file format used for storing the data is NetCDF-4. The NetCDF Climate and Forecast (CF) Metadata Conventions standard names are used for the main variables and global attributes, to ensure compliance with CCI Data Standards [AD-3]. Table 4.9 lists the name, units, dimensions and a description of the data variables. The geostationary products are produced in the format defined for Sentinel 4. This is very similar to that for the polar orbiting products, except that there are no “band 1” specific variables (those with “_uv1” in the table below) - the geostationary sensors do not have measurements in the corresponding spectral range.

Table 4.4: GOME-type RAL data products – List of variables and description. Note that for each variable with "subcolumn" in the name, there is also a corresponding "total_column" variable which contains the corresponding values for the total ozone column.

Variable	Unit	Dimension	Longname / description / comment
latitude	degrees	ground_pixel scanline	Pixel center latitude
longitude	degrees	ground_pixel scanline	Pixel center longitude
latitude_bounds	degrees	ground_pixel scanline	Pixel corner latitude
longitude_bounds	degrees	ground_pixel scanline	Pixel corner longitude
surface_altitude	km	ground_pixel scanline	Surface altitude
snow_ice_flag		ground_pixel scanline	Snow/ice flag
surface_classification		ground_pixel scanline	Surface type
satellite_latitude	degrees	ground_pixel scanline	Satellite latitude
satellite_longitude	degrees	ground_pixel scanline	Satellite longitude
satellite_altitude	km	ground_pixel scanline	Satellite altitude
satellite_orbit_phase		ground_pixel scanline	Satellite orbit phase
geolocation_flags		ground_pixel scanline	L1 Geolocation flags
time	seconds	1	Reference time for which the retrieval is performed
delta_time	milliseconds	scanline	Offset from reference start time of measurement
subcolumn_bounds	hPa	vertices layer	Bounding pressure levels of reported sub columns.
ozone_subcolumn	10^{-6}	layer ground_pixel scanline	Sub-column average mixing ratio of ozone
ozone_subcolumn_precision	10^{-6}	layer ground_pixel scanline	Estimated standard deviation (noise + smoothnig error) of the ozone sub-column average mixing ratio

Variable	Unit	Dimension	Longname / description / comment
qa_value	1	ground_pixel scanline	A continuous quality descriptor; varying between 0 (no data) and 1 (full quality data).
ground_pixel	1	ground_pixel	Ground-pixel index (across-track)
scanline	1	scanline	Scanline index (along-track)
solar_azimuth_angle	degrees	scanline ground_pixel	Solar azimuth angle at the center of each ground pixel
solar_zenith_angle	degrees	scanline ground_pixel	Solar zenith angle at the center of each ground pixel
viewing_azimuth_angle	degrees	scanline ground_pixel	Viewing azimuth angle at the center of each ground pixel
viewing_zenith_angle	degrees	scanline ground_pixel	Viewing zenith angle at the center of each ground pixel
ground_pixel_uv1	1	ground_pixel_uv1	B1 ground-pixel index
scanline_uv1	1	scanline_uv1	B1 scanline index
index_ground_pixel_uv1	1	ground_pixel	Gives B1 ground-pixel index for each B2 ground pixel
index_scanline_uv1	1	scanline	Gives B1 scanline index for each B2 ground pixel
averaging_kernel	1	layer level scanline ground_pixel	Averaging kernels of retrieval. Sensitivity of the retrieved sub-column amount to perturbations in the true ozone profile on a finely resolved vertical grid.
ozone_subcolumn_noise	10^{-6}	layer ground_pixel scanline	Estimated standard deviation from measurement noise of the ozone sub-column average mixing ratio
ozone_subcolumn _number_density_factor	10^{6} mol/m2	layer ground_pixel scanline	Factor to convert sub-column average mixing ratio to number density in mol/m2
cost_function	1	scanline ground_pixel	Solution cost function value
cost_function_uv1	1	scanline_uv1 ground_pixel_uv1	Solution cost function value
cost_function_solar	1	ground_pixel	B1 solar fit cost function
cost_function_solar_uv1	1	ground_pixel_uv1	B2 solar fit cost function
convergence_flag	1	scanline ground_pixel	Convergence flag

Variable	Unit	Dimension	Longname / description / comment
convergence_flag _uv1	1	scanline_uv1 ground_pixel_uv1	Convergence flag
convergence_flag_solar	1	ground_pixel	Convergence flag
convergence_flag_solar_uv 1	1	ground_pixel_uv1	Convergence flag
number_of_steps	1	scanline ground_pixel	Number of retrieval steps
number_of_steps _uv1	1	scanline_uv1 ground_pixel_uv1	Number of retrieval steps
number_of_steps_solar	1	ground_pixel	Number of retrieval steps
number_of_steps_solar_uv 1	1	ground_pixel_uv1	Number of retrieval steps
state_vector	various	state_vector_length scanline ground_pixel	Full retrieval state vector; as retrieved (B2 ozone fit)
state_vector_uv1	various	state_vector_length _uv1 scanline_uv1 ground_pixel_uv1	Full retrieval state vector; as retrieved (B1 ozone fit)
state_vector_solar	various	state_vector_length _solar ground_pixel	Full retrieval state vector; as retrieved (B2 solar fit)
state_vector_solar_uv1	various	state_vector_length _solar_uv1 ground_pixel_uv1	Full retrieval state vector; as retrieved (B1 solar fit)
ozone_subcolumn_uv1	10^{-6}	layer scanline_uv1 ground_pixel_uv1	Sub-column average mixing ratio of ozone from B1 step
ozone_subcolumn_total_ covariance	$(10^{-6})^2$	covariances scanline ground_pixel	Solution covariance matrix of the reported sub columns
ozone_subcolumn_noise _covariance	$(10^{-6})^2$	covariances scanline ground_pixel	Solution covariance matrix of the reported sub columns
processing_quality_flags		scanline ground_pixel	Flags indicating conditions that affect quality of the retrieval.
qa_value		scanline ground_pixel	Overall quality flag
cloud_fraction	1	scanline ground_pixel	Cloud effective radiance fraction used for retrieval
cloud_top_pressure	hPa	scanline ground_pixel	Could effective top pressure
cloud_albedo	1	scanline ground_pixel	Cloud effective albedo used for retrieval
surface_albedo	1	scanline ground_pixel	Surface albedo used for retrieval

Variable	Unit	Dimension	Longname / description / comment
surface_pressure	hPa	scanline ground_pixel	Surface pressure
pressure	hPa	level scanline ground_pixel	Pressure profile
temperature	hPa	level scanline ground_pixel	Temperature profile
ozone_profile_apriori	10^{-6}	level scanline ground_pixel	Apriori ozone profile on fine vertical grid
ozone_subcolumn_apriori	10^{-6}	layer scanline ground_pixel	A priori ozone sub-columns
tropopause_pressure	hPa	scanline ground_pixel	Tropopause pressure

4.1.5 Data volume

An estimate of the file sizes is given in Table 4.11.

Table 4.5: GOME-type RAL data products – Estimates of data volume.

	Month	Year	Full period
GOME	3.5 GB	42 GB	450 GB
GOME-2A	3.5 GB	42 GB	605 GB
GOME-2B	3.5 GB	42 GB	514 GB
GOME-2C	3.5 GB	42 GB	231 GB
OMI	15-28 GB	182-340 GB	7 TB
S5P	150 GB	1.8 TB	12 TB
TEMPO	250 GB	n/a	250 GB
GEMS	80 GB	n/a	80 GB

4.2 UV-visible Merged Ozone Profile (Level-3)

The GOME-type Ozone Profile Essential Climate Variable scheme (GOP-ECV) aggregates, harmonises and merges the ozone retrievals by the RAL level-2 scheme from five UV-visible nadir sounders. This leads to a gridded level-3 data product representing the monthly mean ozone profile between 1995 and 2021.

4.2.1 Used input data

Data from seven UV-visible nadir sensors are considered, starting with GOME in 1995 and continuing to 2024 with several sensors based on an evolved GOME instrument design. For each of these sensors a similar level-2 algorithm was used to maximise consistency of the time series.

Table 4.6: GOP-ECV data product – list of input data sets.

Sensor	Time period	L2 version	Comment
GOME	07/1995 – 12/2004	v03.01	Data from 01/1996 – 06/2011 used for adjustment
SCIAMACHY	05/2003 – 12/2004	v03.00	Data from 01/2005 – 12/2010 used for adjustment
OMI	10/2004 – 10/2021	v02.14	
GOME-2A	01/2007 – 12/2016	v03.00	
GOME-2B	01/2015 – 12/2022	v03.03 (01/2015 – 10/2020); v03.05 (11/2020 – 10/2022)	
GOME-2C	01/2019 – 12/2024	v4.01	
S5P	05/2018 – 12/2024	v4.01	

4.2.2 Resolution and coverage in space and time

Table 4.7 provides an overview of the technical specifications of the GOP-ECV L3 data product. It provides global coverage between surface and 80 km at 4-6 km sampling resolution since 1995. The effective vertical resolution of the retrievals is coarser, about 10-15 km.

Table 4.7: GOP-ECV data product – sampling resolution and coverage in space and time.

Dimension	Specification	Notes
Temporal resolution	monthly	
Temporal coverage	07/1995 – 10/2024	
Horizontal resolution	5° x 5°	
Horizontal coverage	global	except polar night
Vertical resolution	4-6 km	effective retrieval resolution is 10-15 km
Vertical coverage	0-80 km	

4.2.3 Uncertainty estimates, quality indicators, and expected accuracy

The expected quality of GOP-ECV is summarised in Table 4.8.

Table 4.8: Expected quality of GOP-ECV data product.

Quantity	Specification	Notes
Accuracy : systematic component	tbd	pending validation
Accuracy : random component	tbd	pending validation
Stability	tbd	pending validation

4.2.4 Product layers, auxiliary output, format and metadata

The file format used for storing the data is NetCDF-4 classic. The NetCDF Climate and Forecast (CF) Metadata Conventions standard names are used for the main variables and global attributes, to ensure compliance with CCI Data Standards [AD-3]. Table 4.9 lists the name, units, dimensions and a description of the data variables. Table 4.10 presents the included metadata.

Table 4.9: GOP-ECV data product – List of variables and description.

Variable	Unit	Dimension	Longname / description / comment
time	month		Time
latitude	degree N	N_{lat}	Latitude of grid center
longitude	degree E	N_{lon}	Longitude of grid center
pressure	hPa	N_{lev}	Air pressure at layer boundaries
ozone_partial_column	mol m^{-2}	N_{lay} x N_{lat} x N_{lon}	Mole content of ozone in layer
ozone_partial_column_uncertainty	mol m^{-2}	N_{lay} x N_{lat} x N_{lon}	Uncertainty of mole content of ozone in layer
total_ozone_column	mol m^{-2}	N_{lat} x N_{lon}	Vertically integrated ozone_partial_column data

Table 4.10: GOP-ECV data product – List of metadata.

Metadata name	Comment
title	
institution	
project	
history	
product version	
license	
L2_version	
reference	
tracking_id	

Metadata name	Comment
ID	
naming_authority	
keywords	
keywords_vocabulary	
cdm_data_type	
creator_name	
creator_url	
creator_email	
geospatial_lat_min	
geospatial_lat_max	
geospatial_lat_resolution	
geospatial_lat_units	
geospatial_lon_min	
geospatial_lon_max	
geospatial_lon_resolution	
geospatial_lon_units	
geospatial_vertical_min	
geospatial_vertical_max	
time_coverage_start	
time_coverage_end	
time_coverage_duration	
time_coverage_resolution	
time_coverage_list	
standard_name_vocabulary	
date_created	
sensor_list	
platform	
sensor	
key_variables	

4.2.5 Data volume

An estimate of the file sizes is given in Table 4.11.

Table 4.11: GOP-ECV data product – Estimates of data volume.

	Month	Year	Full period
Data volume	0.5 MB	6 MB	165 MB

4.3 IASI Ozone Profile (Level-2)

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 PROFILE ULB-LATMOS CDR was generated at EUMETSAT using the FORLI-O3 retrieval algorithm (v20151001; Hurtmans et al., 2012). The data product consists of 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.

4.3.1 Used input data

TheIASI L2 PROFILE ULB-LATMOS CDR dataset is processed at EUMETSAT for the period 2008-2023 using FORLI-O3 (v20151001) on daily L1C radiances from the IASI sensors on Metop-A, Metop-B and Metop-C. The auxiliary IASI L2 data needed as input to FORLI-O3 were reprocessed by EUMETSAT (with an adapted version of the EUMETSAT operational algorithm V6.6) to produce a homogeneous CDR (Release 1 IASI L2).

Table 4.12: IASI level-2 data products – list of input data sets.

Sensor	Time period	L1 version	Comment
IASI-A	2007 – 2019	2007-2016: reprocessed IASI L1c CDR Release 1; 2017-2019: Operational IASI L1c	http://doi.org/10.15770/EUM_SEC_CLM_0014. This was reprocessed using the version 8.0 of the operational software and used IASI Level 0 data plus the last updated auxiliary files provided by CNES. This release comprises level 1c data from Metop-A satellite for the period ranging from the 10th of July 2007 until the 31st of December 2016. The operational IASI L1c data are used onwards.
IASI-B	2019 – 2023	Operational IASI L1c	https://navigator.eumetsat.int/product/EO:EUM:DAT:METOP:IASIL1C-ALL
IASI-C	2019 – 2023	Operational IASI L1c	https://navigator.eumetsat.int/product/EO:EUM:DAT:METOP:IASIL1C-ALL

4.3.2 Resolution and coverage in space and time

Table 4.13 provides an overview of the technical specifications of the IASI L2 PROFILE ULB-LATMOS CDR data products.

Table 4.13: IASI level-2 data products – sampling resolution and coverage in space and time.

Dimension	Specification	Notes
Temporal resolution	Twice daily	Morning and evening
Temporal coverage	IASI-A: 20080101-20191231; IASI-B: 20191101-20231231; IASI-C: 20191204-20231231	
Horizontal resolution	12 km circle diameter (at nadir); 10 x 20 km^2 (larger viewing angles)	
Horizontal coverage	global	
Vertical resolution	1 km retrieved vertical layers	Effective retrieval resolution is 10-15 km [RD-6]
Vertical coverage	surface - 60 km	

4.3.3 Uncertainty estimates, quality indicators, and expected accuracy

The expected quality of IASI level-2 data is summarised in Table 4.14.

Table 4.14: Expected quality of IASI level-2 data products.

Quantity	Specification	Notes
Accuracy : systematic component	<15% along the profile	Uncertainties of fixed parameters (e.g. temperature profile) - Not taken into account in the total retrieval error matrix.
Accuracy : random component	<35% along the profile	Profile: 10-35% (troposphere), 5-30% (stratosphere, usually <15%); Total columns: < 10% (usually ~3%)
Stability	-0.8%/dec	Drift calculated for IASI-A only [Ozone_cci+_PVIR_5.0]

4.3.4 Product layers, auxiliary output, format and metadata

The file format used for storing the data is NetCDF-4 classic. The NetCDF Climate and Forecast (CF) Metadata Conventions standard names are used for the main variables and global attributes, to ensure compliance with CCI Data Standards [AD-3]. Table 4.15 lists the name, units, dimensions and a description of the data variables. Table 4.16 presents the included metadata.

Table 4.15: IASI level-2 data products – List of variables and description.

Variable	Unit	Dimension	Longname / description / comment
time	Day	N_{time}	UTC observation time in days since 1970-01-01 00:00:00 UTC

Variable	Unit	Dimension	Longname / description / comment
AERIStime	second	N_{time}	UTC observation time in seconds since 1970-01-01 00:00:00 UTC
hour	second	N_{time}	UTC observation hour of the day
minute	minute	N_{time}	UTC observation minute of the hour
second	second	N_{time}	UTC observation second of the minute
latitude	degree north	N_{time}	Latitude of ground pixel center
longitude	degree east	N_{time}	Longitude of ground pixel center
solar_zenith_angle	degree	N_{time}	Solar zenith angle at the Earth's surface for the pixel center
satellite_zenith_angle	degree	N_{time}	Metop zenith angle at the Earth's surface for the pixel center
orbit_number	n/a	N_{time}	Metop orbit number
scanline_number	n/a	N_{time}	Scanline number in the Metop orbit
pixel_number	n/a	N_{time}	Pixel number in the current scanline
ifov_number	n/a	N_{time}	Field of view number in the 2 x 2 observation matrix
retrieval_quality_flag	n/a	N_{time}	Retrieval quality flag summarizing processing flags
surface_altitude	m	N_{time}	Altitude of the surface
Tropopause_altitude	m		Altitude of the tropopause
O3_apriori_partial_column_profile	mol m^{-2}	N_{time} x N_{layers}	Ozone a priori partial column vertical profile in the layers defined by the levels given in the variable atmosphere_pressure_grid
O3_partial_column_profile	mol m^{-2}	N_{time} x N_{layers}	Ozone partial column vertical profile retrieved in the layers defined by the levels given in the variable atmosphere_pressure_grid
O3_partial_column_profile_error	n/a	N_{time} x N_{layers}	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.

Variable	Unit	Dimension	Longname / description / comment
O3_total_degrees_of_freedom	n/a	N_{time}	Degrees of freedom of the signal in the retrieved ozone partial column profile
air_partial_column_profile	mol m^{-2}	N_{time} x N_{layers}	Air partial column vertical profile in the layers defined by the levels given in the variable atmosphere_pressure_grid
atmosphere_pressure_grid	Pascal	N_{time} x $N_{pressures}$	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	(mol m^{-2})/ (mol m^{-2})	N_{time} x N_{layers} x N_{layers}	Ozone partial column averaging kernel matrix in the layers defined by the levels given in the variable atmosphere_pressure_grid.

Table 4.16: IASI level-2 data products – List of metadata.

Metadata name	Comment
Title	IASI/METOP-"X" EUMETSAT CDR ozone (O3) L2 products (profiles)
Institution	ULB-LATMOS for algorithm development ; EUMETSAT for data production ; LATMOS for data extraction and formatting; AERIS for data access
product_version	CDR Release 1 of IASI 2b - 2nd extraction
history	"YYYY-MM-DD hh:mm:ss" (date of data extraction) - Product generated with FORLI v20151001 at EUMETSAT
summary	IASI L2 data were reprocessed by EUMETSAT to product a homogeneous CDR (Climate Data Record). This was the Release 1 IASI L2. The reprocessing was done on Linux using an adapted version of the EUMETSAT operational algorithm V6.6. Until december 2016, the reprocessed Metop-A IASI L1C input data were used (doi:10.15770/EUM_SEC_CLM_0014), after this date and for Metop-B the operational IASI L1c were used. ERA5 were used as auxiliary model data. This dataset contains Level 2 ozone profile products from IASI observations as that is done from OZO EUMETSAT IASI L2 files (data reconstruction and formatting in netcdf files are processed by LATMOS);

Metadata name	Comment
Source	EUMETSAT IASI Level 2 ozone (O3) release 1
References	Reference to the O3 retrieval: FORLI radiative transfer and retrieval code for IASI, J. Quant. Spectrosc. Ra., 113, 1391-1408, https://doi.org/10.1016/j.jqsrt.2012.02.036
id	IASI_METOP"A or B"_L2_O3_PROFILE_"yyyymmdd"_EUMETSAT_CDR_"version".nc
Tracking_id	
geospatial_lat_min	-90.0
geospatial_lat_max	+90.0
geospatial_latitude_units	Degree north
geospatial_lon_min	-180.0
geospatial_lon_max	+180.0
geospatial_longitude_units	Degree east
geospatial_vertical_min	0
geospatial_vertical_max	60
Geospatial_vertical_units	km
time_coverage_start	
time_coverage_end	
conventions	CF-1.8
standard_name_vocabulary	NetCDF Climate and Forecast (CF) Medata Convention version 80, 7 February 2022
platform	Metop-“X”
sensor	IASI
spatial_resolution	12km at nadir
creator_type	institution
creator_name	ULB-LATMOS
contact_email	contact form at http://iasi.aeris-data.fr/contact/
data_policy	see https://iasi.aeris-data.fr/data-use-policy/

4.3.5 Data volume

An estimate of the file sizes is given in Table 4.17. At the time of writing (Oct 2023), four days of IASI data per month are expected for release by the end of the current phase of CCI+.

Table 4.17: IASI level-2 data products – Estimates of data volume, representing a subsample of 3.5 prixels on 10 prixels.

	Month	Year	Full period
Data volume (All days but 3.5/10 pixels)	~45 GB per IASI sensor	~550 GB per IASI sensor	IASI-A : ~6.5 TB; IASI-B : ~2.4 TB; IASI-C: ~2.3 TB

4.4 IASI Merged Ozone Profile (Level-3)

The merged IASI profile product combines data retrieved from the three IASI sensors. Take note that the Level-2 data version used is not that the version described in the previous section. It consists of daily partial columns profiles in 1° latitude x 1° longitude bins between surface and 60 km.

4.4.1 Used input data

The IASI merged Level-3 ozone profile dataset is generated by ULB-LATMOS using daily Level-2 IASI-A (20080101-20190919), IASI-B (20130308-20231231) and IASI-C (20190920-20231231) ozone profiles. The Level-2 data were generated by ULB with FORLI-O3 v20191122 (Hurtmans et al., 2012).

Table 4.18: IASI merged level-3 data product – list of input data sets.

Sensor	Time period	L2 version	Comment
IASI-A	01/2008 – 09/2019	FORLI-O3 v20191122	Processed at ULB
IASI-B	03/2013 – present	FORLI-O3 v20191122	Processed at ULB
IASI-C	09/2019 – present	FORLI-O3 v20191122	Processed at ULB

4.4.2 Resolution and coverage in space and time

Table 4.19 provides an overview of the technical specifications of the IASI data product.

Table 4.19: IASI merged level-3 data product – sampling resolution and coverage in space and time.

Dimension	Specification	Notes
Temporal resolution	daily	Morning & evening orbits combined
Temporal coverage	20080101 - 20231231	IASI-A: 20080101-20130307; IASI-A &-B: 20130308-20190919; IASI-B & -C: 20190920-20231231
Horizontal resolution	1° x 1°	
Horizontal coverage	global	
Vertical resolution	1 km retrieved vertical layers	Effective retrieval resolution is 10-15 km [RD-6]
Vertical coverage	surface - 60 km	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)

4.4.3 Uncertainty estimates, quality indicators, and expected accuracy

The expected quality of IASI merged is summarised in Table 4.20.

Table 4.20: Quality of IASI merged level-3 data products.

Quantity	Specification	Notes
Accuracy : systematic component	<15% along the profile	Uncertainties of fixed parameters (e.g. temperature profile) are not taken into account in the total retrieval error matrix.
Accuracy : random component	<35% along the profile	Profile: 10-35% (troposphere), 5-30% (stratosphere, usually <15%); Total columns: < 10% (usually ~3%)
Stability	< -0.6 ± 0.1%/decade	Very low drifts within the product requirements; the merged IASI integrated total ozone is temporally very stable [Ozone_cci+_PVIR_5.0]

4.4.4 Product layers, auxiliary output, format and metadata

The file format used for storing the data is NetCDF-4 classic. The NetCDF Climate and Forecast (CF) Metadata Conventions standard names are used for the main variables and global attributes, to ensure compliance with CCI Data Standards [AD-3]. Table 4.21 lists the name, units, dimensions and a description of the data variables. Table 4.22 presents the included metadata.

Table 4.21: IASI merged level-3 data product – List of variables and description.

Variable	Unit	Dimension	Longname / description / comment
latitude	degree N	N_{lat}	Center of latitude bins: -89.5°: 1°:89.5°
longitude	degree E	N_{lon}	Centers of longitude bins: -179.5°:1°:179.5°
surface_altitude	km	N_{lat} x N_{lon}	Mean surface altitude in 1°x1° bin
atmosphere_pressure_grid	Pascal	N_{lat} x N_{lon} x $N_{pressures}$	Mean pressures corresponding to retrieval layers boundaries in bins
O3_total_column	mol m^{-2}	N_{lat} x N_{lon}	Merged integrated total O3 columns in mole/m2, calculated as the weighted average of all values assigned to the 1°x1° bin
O3_total_column_error	mol m^{-2}	N_{lat} x N_{lon}	Uncertainty in mole/m2 associated with the weighted average of integrated total O3 columns in the 1°x1° bin and calculated as the reciprocal square root of the sum of all the individual weights
O3_partial_column_profile	mol m^{-2}	N_{lat} x N_{lon} x N_{layers}	Merged ozone partial column vertical profile in mole/m2 retrieved in the layers defined by the levels given in the variable atmosphere_pressure_grid. It is calculated as the weighted average of all values assigned to the 1°x1° bin and for each layer

Variable	Unit	Dimension	Longname / description / comment
O3_partial_column_error_profile	mol m^{-2}	N_{lat} x N_{lon} x N_{layers}	Uncertainty in mole/m2 associated with the weighted average of O3 partial column vertical profile in the 1°x1° bin and for each layer. It is calculated as the reciprocal square root of the sum of all the individual weights.
O3_apriori_partial_column_profile	mol m^{-2}	N_{lat} x N_{lon} x N_{layers}	O3 a priori partial column vertical profile in mole/m2 in the 1°x1° bin, corresponding to the layers defined by the levels given in the variable atmosphere_pressure_grid.
air_partial_column_profile	mol m^{-2}	N_{lat} x N_{lon} x N_{layers}	Merged air partial column vertical profile in the layers defined by the levels given in the variable atmosphere_pressure_grid and calculated as the weighted average of all values assign ed to the 1°x1° bin and for each layer
O3_total_column_averaging_kernel	mol.m-2/mol.m-2	N_{lat} x N_{lon} x N_{layers}	Merged ozone total column averaging kernel ((mol/m^2)/(mol/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.

Table 4.22: IASI merged level-3 data product – List of metadata.

Metadata name	Comment
Title	L3 Nadir IASI-A, -B, -C Merged Ozone Profile
Institution	ULB for algorithm development and data production
product_version	L3 IASI merged O3 - Release 1.0
Source	IASI Level-2 FORLI-O3 v20191122
Source_retrieval_method	Optimal Estimation with one constant a priori (profile and covariance matrix)
Source_retrieval_algorithm	FORLI-O3, v20191122
source_references	Reference to the FORLI-O3 retrieval: FORLI radiative transfer and retrieval code for IASI, J. Quant. Spectrosc. Ra., 113, 1391-1408, https://doi.org/10.1016/j.jqsrt.2012.02.036, 2012
sensors	IASI/Metop-A (OCT 2007 - OCT 2021), IASI/Metop-B (MAR 2013 - now) & IASI/Metop-C (SEP 2019 - now)
sensor_merged_periods	IASI-A: 20080101 - 20130307; IASI-A & -B: 20130308 - 20190919; IASI-B & -C: 20190920 - now
id	IASI_FORLI_O3_MERGED_YYYYMMDD_V1.0.nc
creator_name	ULB-LATMOS
creator_email	Catherine.wespes@ulb.be

Metadata name	Comment
geospatial_lat_min	-90 deg
geospatial_lat_max	90 deg
geospatial_lat_resolution	1 deg
geospatial_latitude_units	degree_north
geospatial_lon_min	-180 deg
geospatial_lon_max	180 deg
geospatial_longitude_resolution	1
geospatial_longitude_units	degree_east
geospatial_vertical_range	Surface - 60 km
geospatial_vertical_resolution	1 km from surface to 40 km, with one extra layer from 40 to 60 km
retrieval_quality_flags	A posteriori general retrieval quality flag summarizing processing flags is applied on IASI L2 O3 products before merging; it is based on a combination of processing flags (negative altitude, large cloud fraction, residuals biased or sloped, large RMS, suspect AK, max number of iteration exceeded, low DOFS, etc)
value_for_nodata	NaN
Project_Name	O3-CCI+ Phase-3

4.4.5 Data volume

An estimate of the file sizes is given in Table 4.23.

Table 4.23: IASI merged level-3 data product– Estimates of data volume.

	Month	Year	Full period
Data volume	4 GB	47 GB	755 GB

5 Limb profile

5.1 OMPS-NOAA21 Ozone Profiles

5.1.1 Used input data

The OMPS-NOAA21 L2 data set has been processed at IUP-UB using the SCIATRAN radiative transfer model. The sensor was launched at the end of 2022 and L1 data are available from February 2023.

Table 6.1: OMPS-NOAA21 level-2 data product – input data set.

Sensor	Time period	L1 version	Comment
OMPS-NOAA21	2023 – 2025	First version released by NASA including pointing corrections (v1.0).	This is the second L2 processing version after the product released in Phase II.

5.1.2 Resolution and coverage in space and time

Table 6.2 provides an overview of the technical specifications of the OMPS-NOAA21 data product.

Table 6.2: OMPS-NOAA21 level-2 data product – sampling resolution and coverage in space and time.

Dimension	Specification	Notes
Temporal resolution	One measurement every 15s, about 200 observation per orbit	Change of resolution in December 2023, increased to one measurement every 8s
Temporal coverage	Feb 2023 - present	
Horizontal resolution	~200 km along track, 3 km across track	
Horizontal coverage	Global (81°S – 81°N)	
Vertical resolution	1 km retrieved vertical layers	Effective retrieval resolution is 2-3 km
Vertical coverage	8.5 (or cloud top height) – 60.5 km	

5.1.3 Uncertainty estimates, quality indicators, and expected accuracy

The expected quality of OMPS-NOAA21 L2 data is summarised in Table 6.3.

Table 6.3: Expected quality of OMPS-NOAA2 L2 data.

Quantity	Specification	Notes
Estimated systematic component	<5% along the profile	Estimated for OMPS-NPP retrievals in a dedicated study.
Retrieval noise	Within 2-3 % between 20 and 50 km, increasing up to 10 % in the UTLS.	
Stability	To be investigated	Possibly too short a time series to assess its stability.

5.1.4 Product layers, auxiliary output, format and metadata

Data are stored in the classic NetCDF-4 data format. The NetCDF Climate and Forecast (CF) Metadata Conventions standard names are used for the main variables and global attributes, to ensure compliance with CCI Data Standards [AD-3]. Table 6.4 lists the name, units, dimensions and a description of the data variables. Table 4.165 presents the included metadata.

Table 6.4: OMPS-NOAA21 L2 data product – List of variables and description.

Variable	Unit	Dimension	Longname / description / comment
altitude	Km	$N_{altitude}$	Altitude grid
time	days	N_{time}	Days since 1900-01-01 00:00:00 UTC
string_time	String	N_{time}	Time string in YYYYMMDDThhmmssZ
latitude	degree N	N_{time}	Latitude of tangent point at 25 km
longitude	degree E	N_{time}	Longitude of tangent point at 25 km
orbit_number	n/a	N_{time}	Metop orbit number
FOV_number	n/a	N_{time}	Profile number in the current scanline
PMC_flag	n/a	N_{time}	Polar mesospheric cloud flag
O3_concentration	mol m^{-3}	N_{time} x $N_{altitude}$	Ozone retrieved vertical profile on the altitude grid defined by the altitude variable
O3_concentration_standard_error	mol m^{-3}	N_{time} x $N_{altitude}$	Retrieval error
pressure	hPa	N_{time} x $N_{altitude}$	Pressure information from ECMWF interpolated at the altitude grid
stratospheric_ozone_column	mol m^{-2}	N_{time}	Stratospheric column from the tropopause height

Variable	Unit	Dimension	Longname / description / comment
temperature_ecmwf	K	N_{time} x $N_{altitude}$	Temperature information from ECMWF interpolated at the altitude grid
tropopause_altitude	km	N_{time}	Thermal tropopause altitude from ECMWF according to WMO definition
tropopause_altitude_second	km	N_{time}	Thermal tropopause altitude from ECMWF according to WMO definition, second occurrence
vertical_resolution	km	N_{time} x $N_{altitude}$	Vertical resolution of the retrieved profiles.

Table 6.5: OMPS-NOAA21 L2 data product – List of metadata.

Metadata name	Comment
Affiliation	IUP - University of Bremen
Comment	These data were produced at the University of Bremen as part of the ESA OZONE CCI project
creator_address	Otto-Hahn-Allee 1, D-28359, Bremen, Germany
creator_email	carloarosio@iup.physik.uni-bremen.de
creator_name	Carlo Arosio
creator_url	www.iup.uni-bremen.de
conventions	CF-1.6
file_version	fv0002
file_version_description	Second version of the retrieval
format_version	CCI Data Standard v2.3
geospatial_lat_min	-81.3
geospatial_lat_max	81.3
geospatial_lat_resolution	
geospatial_lat_units	degrees_north
geospatial_lon_min	-180
geospatial_lon_max	180
geospatial_longitude_resolution	
geospatial_longitude_units	degrees_east
geospatial_vertical_min	65.0 km
geospatial_vertical_max	5.0 km
id	
institution	IUP-UB
keywords	satellite, observation, atmosphere, ozone, level 2

Metadata name	Comment
keywords_vocabulary	GCMD Science Keywords
history	Original product generated by NASA
level_1_data_versions	v1.0
license	ESA CCI data policy: free and open access
platform	NOAA 21
product_version	L2 V2_0
references	www.esa-ozone-cci.org

5.1.5 Data volume

An estimate of the file sizes is given in Table 6.6, accounting for 2 years of data.

Table 6.6: OMPS-NOAA21 level-2 data product – Estimates of data volume.

	Month	Year	Full period
Data volume	~0.1 GB	~1.0 GB	~2.0 GB

5.2 Merged OMPS product

5.2.1 Used input data

Level-2 profile data from the two OMPS-LP instruments, onboard Suomi NPP and NOAA-21 are merged into a L3 gridded data set covering the period 2012-present. The merging was performed on deseasonalized anomalies and the time series reconstructed adding the average seasonal cycle of the two instruments. The gridding is on a monthly basis, with a 5° latitude x 20° longitude binning and a 1.5 km vertical sampling.

Table 5.1: OMPS merged data product – list of input data sets.

Sensor	Time period	L2 version	Comment
OMPS-LP / SNPP	2012 – present	IUP-UB v4.0	Onboard Suomi-NPP
OMPS-LP / N21	2023 – present	IUP-UB v2.0	Onboard NOAA 21

5.2.2 Resolution and coverage in space and time

Table 5.7 provides an overview of the technical specifications of the OMPS merged level-3 data product.

Table 5.2: OMPS merged data product – sampling resolution and coverage in space and time.

Dimension	Specification	Notes
Temporal resolution	monthly	
Temporal coverage	2012-2025	
Horizontal resolution	5° latitude x 20° longitude	
Horizontal coverage	Global (81°S – 81°N)	
Vertical resolution	2-3 km	The vertical sampling is 1 km
Vertical coverage	8.5 – 60.5 km	

5.2.3 Uncertainty estimates, quality indicators, and expected accuracy

TBD

5.2.4 Product layers, auxiliary output, format and metadata

The file format used for storing the data is NetCDF-4 classic. The NetCDF Climate and Forecast (CF) Metadata Conventions standard names are used for the main variables and global attributes, to ensure compliance with CCI Data Standards [AD-3]. Table 5.9 lists the name, units, dimensions and a description of the data variables. Table 5.10 presents the included metadata.

Table 5.3: OMPS merged data product – List of variables and description.

Variable	Unit	Dimension	Longname / description / comment
time			string DD-MM-YYYY
altitude	Km	N_{alt}	Altitude grid
latitude	degree N	N_{lat}	
longitude	degree E	N_{lon}	
pressure	hPa	N_{lon} x N_{lat} x N_{alt}	pressure profiles from ERA-5
temperature	K	N_{lon} x N_{lat} x N_{alt}	temperature profiles from ERA-5
ozone_number_density	mol cm^{-3}	N_{lon} x N_{lat} x N_{alt}	interpolated ozone profiles from satellites.
ozone_number_densitiy_std	mol cm^{-3}	N_{lon} x N_{lat} x N_{alt}	random uncertainty of merged ozone profiles
ozone_anomalies	%	N_{lon} x N_{lat} x N_{alt}	Relative ozone anomalies
ozone_anomalies_uncertainty	%	N_{lon} x N_{lat} x N_{alt}	Random uncertainty of ozone anomalies
tropopause_altitude	Km	N_{lon} x N_{lat}	Thermal tropopause from ERA-5 according to WMO definition

Table 5.4: OMPS merged data product – List of metadata.

Metadata name	Comment
title	OMPS merged
institution	IUP-UB
source	Ozone profiles from OMPS-LP onboard Suomi NPP and NOAA-21 platforms.
creator_name	Carlo Arosio
creator_email	carloarosio@iup.physik.uni-bremen.de
geospatial_lat_resolution	5°
geospatial_lon_resolution	20°
geospatial_lat_min	81° S
geospatial_lat_max	81° N
geospatial_lon_min	-180°
geospatial_lon_max	180°
geospatial_vertical_min	12.5 km
geospatial_vertical_max	60.5 km
value_for_nodata	NaN

5.2.5 Data volume

An estimate of the file sizes is given in Table 5.11.

Table 5.5: OMPS merged data product – Estimates of data volume.

	Month	Year	Full period
Data volume	0.1 MB	1 MB	10 MB

5.3 High-resolution Gap-free Merged Ozone Profile (Level-3)

The vertical distribution of ozone can be retrieved at relatively high resolution from measurements in the UV-visible, IR and MW spectral ranges at Earth's limb. Combining ozone fields by the SILAM Chemistry Transport Model and observations from eight limb/occultation sounders a gap-free gridded ozone profile product is developed with high horizontal (1° x 1°) and temporal (daily) resolution, covering the entire atmosphere.

5.3.1 Used input data

Level-2 profile data from eight limb and occultation sounders are used. For OMPS-LP, two profile products are considered. All profile data are taken from the updated HARMOZ database

maintained by the CCI team [RD-5]. Meteorological data required to convert the profile representation to from altitude/number density to pressure/volume mixing ratio are either retrieved by the sensor or taken from ECMWF's ERA5 reanalysis [RD-7]**Error! Reference source not found.**.

Table 5.6: LIMB-HIRES data product – list of input data sets.

Sensor	Time period	L2 version	Comment
Aura MLS	2004 – present	NASA v5	
GOMOS	2002 – 2012	ALGOM2S v1	
MIPAS	2002 – 2012	KIT v8	
SCIAMACHY	2002 – 2012	IUP-UB v3.5	
OSIRIS	2001 – present	USask v7.4	
OMPS-LP	2012 – present	USask v1.3.0	
OMPS-LP	2012 – present	IUP-UB v4.1	
SAGE III/ISS	2017 – present	NASA v6.0	
ACE-FTS	2004 – present	V5.2	

5.3.2 Resolution and coverage in space and time

Table 5.7 provides an overview of the technical specifications of the LIMB-HIRES level-3 data product. This data product combines information from multiple limb sounders. An extended profile is provided as well, filling in the lower part of the profiles with ozone by the SILAM chemistry-transport model.

Table 5.7: LIMB-HIRES data product – sampling resolution and coverage in space and time.

Dimension	Specification	Notes
Temporal resolution	daily	
Temporal coverage	2001 – present	
Horizontal resolution	1°x1°	
Horizontal coverage	global	
Vertical resolution	1-2 km	
Vertical coverage	900-0.02 hPa	lower part from SILAM CTM

5.3.3 Uncertainty estimates, quality indicators, and expected accuracy

The expected quality of LIMB-HIRES is summarised in Table 5.8.

Table 5.8: Expected quality of LIMB-HIRES data product.

Quantity	Specification	Notes
Accuracy : systematic component	As for Aura MLS	Profiles from other sensors are debiased with respect to Aura MLS

Quantity	Specification	Notes
Accuracy : random component	~3% at 20-40 km, increasing at lower and upper altitudes	
Stability	As for Aura MLS	Profiles from other sensors are debiased with respect to Aura MLS

5.3.4 Product layers, auxiliary output, format and metadata

The file format used for storing the data is NetCDF-4 classic. The NetCDF Climate and Forecast (CF) Metadata Conventions standard names are used for the main variables and global attributes, to ensure compliance with CCI Data Standards [AD-3]. Table 5.9 lists the name, units, dimensions and a description of the data variables. Table 5.10 presents the included metadata.

Table 5.9: LIMB-HIRES data product – List of variables and description.

Variable	Unit	Dimension	Longname / description / comment
time			string DD-MM-YYYY
latitude	degree N	N_{lat}	
longitude	degree E	N_{lon}	
pressure_sat	hPa	N_{lev_sat}	pressure levels for satellite data
pressure_ext	hPa	N_{lev_ext}	pressure levels extended into troposphere
ozone_satellite	mol m^{-3}	N_{lon} x N_{lat} x N_{lev_sat}	interpolated ozone profiles from satellites. Conversion factor to DU/km is provided.
ozone_satellite_error	mol m^{-3}	N_{lon} x N_{lat} x N_{lev_sat}	random uncertainty of interpolated ozone profiles from satellites
ozone_extended	mol m^{-3}	N_{lon} x N_{lat} x N_{lev_ext}	interpolated ozone profiles from satellites with extension to troposphere with SILAM data. Conversion factor to DU/km is provided
ozone_extended_error	mol m^{-3}	N_{lon} x N_{lat} x N_{lev_ext}	random uncertainty of interpolated ozone profiles from satellites with extension to troposphere with SILAM data

Table 5.10: LIMB-HIRES data product – List of metadata.

Metadata name	Comment
Title	L3 Limb Merged Gap-free High-resolution Ozone Profiles
Institution	Finnish Meteorological Institute
Source	Ozone profiles from MLS, GOMOS, SCIAMACHY, MIPAS, OSIRIS, ACE-FTS, OMPS-LP, SAGE III/ISS, simulations by SILAM CTM
History	Original development: SUNLIT project (2020); further development: CCI+ (2023).
creator_name	
creator_email	
geospatial_lat_resolution	1 deg
geospatial_lon_resolution	2 deg
geospatial_lat_min	-88 deg
geospatial_lat_max	88 deg
geospatial_lon_min	-180 deg
geospatial_lon_max	180 deg
geospatial_vertical_min	900 hPa
geospatial_vertical_max	0.02 hPa
value_for_nodata	NaN

5.3.5 Data volume

An estimate of the file sizes is given in Table 5.11.

Table 5.11: LIMB-HIRES data product – Estimates of data volume.

	Month	Year	Full period
Data volume	2 GB	24 GB	500 GB

5.4 SAGE-CCI-OMPS+

The original version of the merged SAGE-CCI- OMPS dataset was created in 2017 (Sofieva et al., 2017). Then, in Phase 1 of Ozone_cci+ project, it was updated by including more individual datasets, this version is called SAGE-CCI-OMPS+ dataset (Sofieva et al., 2023). In Phase 3 of Ozone_cci project, also OMPS-LP data processed by NASA will be included into the merged dataset.

5.4.1 Used input data

Level-2 profile data from nine limb and occultation sounders are used. For OMPS-LP, three profile products are considered. All profile data are taken from the updated HARMOZ database maintained by the CCI team [RD-5].

Table 5.12: SAGE-CCI-OMPS+ data product – list of input data sets.

Sensor	Time period	L2 version	Comment
SAGE II	1984 – 2005	NASA v7	
GOMOS	2002 – 2012	ALGOM2S v1	
MIPAS	2002 – 2012	KIT v8	
SCIAMACHY	2002 – 2012	IUP-UB v3.5	
OSIRIS	2001 – present	USask v7.3	
OMPS-LP/SNPP	2012 – present	USask v1.3.0	
OMPS-LP/SNPP	2012 – present	IUP-UB v4.1	
OMPS-LP/SNPP	2012-present	NASA v2.6	
SAGE III/ISS	2017 – present	NASA v5.3	
ACE-FTS	2004 – present	UoT v5	
POAM III	1998 – 2005	NRL v4	

5.4.2 Resolution and coverage in space and time

Table 5.13 provides an overview of the technical specifications of the merged SAGE-CCI-OMPS+ data product. This data product combines information from multiple limb sounders.

Table 5.13: SAGE-CCI-OMPS+ data product – sampling resolution and coverage in space and time.

Dimension	Specification	Notes
Temporal resolution	monthly	
Temporal coverage	1984 – present	
Horizontal resolution	10° latitude bins	
Horizontal coverage	global	
Vertical resolution	1 km	
Vertical coverage	10-50 km	

5.4.3 Uncertainty estimates, quality indicators, and expected accuracy

The expected quality of SAGE-CCI-OMPS+ is summarised in Table 5.14.

Table 5.14: Expected quality of SAGE-CCI-OMPS+ dataset.

Quantity	Specification	Notes
Accuracy : systematic component		The main dataset is merged deseasonalized anomalies For absolute values: amplitude of seasonal cycle is from MIPAS measurements, Absolute values are the mean on OSIRIS and SAGE II in overlapping periods.
Accuracy : random component	below 1% in the stratosphere, 1-7 % in the UTLS	See ATBD and CECR for information on uncertainty estimation
Stability	expected to be stable	The merging is via computing the median of deseasonalized anomalies. This ensures low sensitivity to potential drifts

5.4.4 Product layers, auxiliary output, format and metadata

All data are included in one netcdf4 file, its main parameters are collected in Table 5.16.

Table 5.15: 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, 8- SAGE III/ISS, 9- POAM III
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

	Parameter	Unit	Dimension	Description
	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	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

5.4.5 Data volume

The size of SAGE-CCI-OMPS+ dataset is 62 MB.

5.5 MEGRIDOP

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.

The detailed description of the merging method can be found in (Sofieva et al., 2021).

5.5.1 Used input data

Level-2 profile data from six limb and occultation sounders are used. For OMPS-LP, three profile products are considered. All profile data are taken from the updated HARMOZ database maintained by the CCI team [RD-5].

Table 5.16: MEGRIDOP data product – list of input data sets.

Sensor	Time period	L2 version	Comment
GOMOS	2002 – 2012	ALGOM2S v1	
MIPAS	2002 – 2012	KIT v8	
SCIAMACHY	2002 – 2012	IUP-UB v3.5	
OSIRIS	2001 – present	USask v7.3	
OMPS-LP/SNPP	2012 – present	USask v1.3.0	
OMPS-LP/SNPP	2012 – present	IUP-UB v3.3	
OMPS-LP/SNPP	2012 – present	NASA v2.6	
MLS	2004 – present	NASA v5	

5.5.2 Resolution and coverage in space and time

Table 5.17 provides an overview of the technical specifications of the merged MEGRIDOP data product. This data product combines information from multiple limb sounders.

Table 5.17: MEGRIDOP dataset – sampling resolution and coverage in space and time.

Dimension	Specification	Notes
Temporal resolution	monthly	
Temporal coverage	1984 – present	
Horizontal resolution	10° latitude x 20° longitude	
Horizontal coverage	global	
Vertical resolution	1 km	
Vertical coverage	10-50 km	

5.5.3 Uncertainty estimates, quality indicators, and expected accuracy

The expected quality of MEGRIDOP is summarised in Table 5.18.

Table 5.18: Expected quality of MEGRIDOP dataset.

Quantity	Specification	Notes
Accuracy : systematic component		The main dataset is merged deseasonalized anomalies For absolute values: amplitude of seasonal cycle is from MIPAS measurements, Absolute values are the mean on OSIRIS and SAGE II in overlapping periods.
Accuracy : random component	below 1% in the stratosphere, 1-7 % in the UTLS	See ATBD and CECR for information on uncertainty estimation
Stability	expected to be stable	The merging is via computing the median of deseasonalized anomalies. This ensures low sensitivity to potential drifts

5.5.4 Product layers, auxiliary output, format and metadata

The MEGRIDOP dataset is provided in one NetCDF-4 file.

Table 5.19: The variables in MEGRIDOP 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	$N_{date}\times1$	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°
	longitude_centers	degree_east	$N_{lon}\times1$	Centers of longitude bins: -170°:20°:170°
	Instruments	-	$N_{instru}\times1$	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 datasets	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
	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

5.5.5 Data volume

The size of the MEGRIDOP dataset is 810 MB.

5.6 LIMB-UTLS

5.6.1 Used input data

Level-2 profile data from eight limb and occultation sounders are used. For OMPS-LP, three profile products are considered. All profile data are taken from the updated HARMOZ database maintained by the CCI team [RD-5].

Table 5.20: LIMB-UTLS data product – list of input data sets.

Sensor	Time period	L2 version	Comment
SAGE II	1984 – 2005	NASA v7	
GOMOS	2002 – 2012	ALGOM2S v1	
MIPAS	2002 – 2012	KIT v8	
SCIAMACHY	2002 – 2012	IUP-UB v3.5	
OSIRIS	2001 – present	USask v7.3	
OMPS-LP/SNPP	2012 – present	USask v1.3.0	
OMPS-LP/SNPP	2012 – present	IUP-UB v4.1	
OMPS-LP/SNPP	2012 – present	NASA v2.6	
SAGE III/ISS	2017 – present	NASA v5.3	
ACE-FTS	2004 – present	UoT v5	

5.6.2 Resolution and coverage in space and time

Table 5.21 provides an overview of the technical specifications of the merged LIMB-UTLS data product. This data product combines information from multiple limb sounders.

Table 5.21: LIMB-UTLS dataset – sampling resolution and coverage in space and time.

Dimension	Specification	Notes
Temporal resolution	monthly	
Temporal coverage	1984 – present	
Horizontal resolution	10° latitude	
Horizontal coverage	global	
Vertical resolution	1 km (TBD)	
Vertical coverage	from 5 km below to 10 km above the tropopause	

5.6.3 Uncertainty estimates, quality indicators, and expected accuracy

The expected quality of LIMB-UTLS is summarised in Table 5.22

Table 5.22: Expected quality of the LIMB-UTLS dataset.

Quantity	Specification	Notes
Accuracy : systematic component		The main dataset is merged deseasonalized anomalies. Also absolute values are provided by restoring the seasonal cycle.
Accuracy : random component	1-7 % in the UTLS	See ATBD and CECR for information on uncertainty estimation
Stability	expected to be stable	The merging is via computing the median of deseasonalized anomalies. This ensures low sensitivity to potential drifts. A better stability in the UTLS is expected compared to the SAGE-CCI-OMPS+ dataset

5.6.4 Product layers, auxiliary output, format and metadata

All data are included in one netcdf4 file, its main parameters are collected in Table 5.23.

Table 5.23: The variables of the LIMB-UTLS 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 relative to the tropopause
	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, 8- SAGE III/ISS
Merged data	merged_ozone_anomaly	%	$N_{date}\times N_{alt}\times N_{lat}$	Merged deseasonalized anomalies
	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
	tropopause_pressure	hPa	$N_{date}\times N_{alt}\times N_{lat}$	Mean tropopause pressure corresponding to spatiotemporal bins

	Parameter	Unit	Dimension	Description
	tropopause_height	km	$N_{date} \times N_{alt} \times N_{lat}$	Mean tropopause height corresponding to spatiotemporal bins
Individual	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

6 References

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