Ozone_cci+

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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

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 second phase of the Ozone_cci+ project (2022-2024). 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 Requirement Document, Ozone_cci+_URD_4.1, Issue 4, Revision 1, March 2025. Available at https://climate.esa.int/en/projects/ozone/key-documents.

[RD-4] ATBD, Ozone CCI+ Algorithm Theoretical Basis Document, Ozone_cci+_D2p1_ATBD_v3.2, Issue 3, Revision 2, March 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+_PVIR_5.2, 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 Total ozone

The Multi-Sensor Reanalysis 2 (MSR2) data product provides monthly mean total ozone columns (TC identifier) at 0.5° x 0.5° horizontal resolution since 1960. It is generated from the assimilation of level-2 total ozone column data by 19 UV-visible nadir sounders and the ground-based Dobson network.

2.2 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. Two gridded products are planned, 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.

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).

2.3 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 four sensors (OMI, 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 (though subsampled to 3-10 days per month).

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 on 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 are combined in a daily 1° x 1° gridded ozone profile product, starting in 2008.

2.4 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]. One merged profile data product is being developed that combines homogenised ozone data from eight limb sensors (Aura MLS, OSIRIS, GOMOS, MIPAS, SCIAMACHY, ACE-FTS, OMPS-LP, SAGE III/ISS) and information from the SILAM model. This product is gap-free and represents daily gridded mean ozone profile between surface and 0.02 hPa at 1° x 1° horizontal resolution since 2001.

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. Data sets marked in red are still in development phase and will not be publicly released.

Product identifier	Source / processing center	Proc-essing level	Time		Vertical		Horizontal	
			Coverage	Resolution	Coverage	Resolution	Coverage	Resolution
Total ozone								
TC_L4_MSR	KNMI	L4	1960-2022	monthly	sfc - TOA	n/a	global	0.5° x 0.5°
Tropospheric ozone								
TRC_L3_GTTO_ECV	DLR	L3	1995-2023	monthly	sfc - 270 hPa	n/a	20°S – 20°N	1° x 1°
TRC_L3_GTO_LIMB	FMI	L3	2004-2023	monthly	sfc - LRT km	n/a	88°S – 88°N	1° x 1°
TRC_L3_OMI_LIMB	FMI	L3	2004-2023	monthly	sfc - LRT km	n/a	88°S – 88°N	1° x 1°
Nadir profile								
NP_L2_GOME2B	RAL	L2	2013-2023	daily	0-80 km	4-6 km	global	160 km x 160 km
NP_L2_GOME2C	RAL	L2	2019-2023	daily	0-80 km	4-6 km	global	160 km x 160 km
NP_L2_OMI	RAL	L2	2004-2023	daily	0-80 km	4-6 km	global	50 km x 50 km
NP_L2_S5P	RAL	L2	2018-2023	daily	0-80 km	4-6 km	global	15 km x 38 km
NP_L3_GOP_ECV	DLR	L3	1995-2021	monthly	0-80 km	4-6 km	global	5° x 5°
NP_L2_IASIA	ULB/EUM	L2	2008-2019	daily	0-60 km	1 km	global	10 km x 20 km
NP_L2_IASIB	ULB/EUM	L2	2013-2023	daily	0-60 km	1 km	global	10 km x 20 km
NP_L2_IASIC	ULB/EUM	L2	2019-2023	daily	0-60 km	1 km	global	10 km x 20 km
NP_L3_IASI_MRG	ULB	L3	2008-2023	daily	0-60 km	1 km	global	1° x 1°
Limb profile								
LP_L3_HIRES	FMI	L3	2002-2023	monthly	900-0.02 hPa	1 km		

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

3 Total ozone

3.1 Multi-Sensor Reanalysis 2 (Level-4)

The Multi-Sensor Reanalysis 2 (MSR2) data product is a multi-decadal level-4 (i.e. assimilation-based) total ozone column data record based on observations by 19 nadir sensors in the near-ultraviolet Huggins band (since the 1970s) and by the ground-based Dobson instrument network (since the 1960s), and the TMDAM assimilation scheme with detailed error modelling. The MSR2 data product provides monthly mean total ozone columns at 0.5° x 0.5° horizontal resolution since 1960.

3.1.1 Used input data

The assimilation scheme ingests total ozone column data by 19 UV-visible nadir sensors, starting with BUV-Nimbus4 launched in 1970. Ground-based observations by Dobson instruments are assimilated prior to the introduction of TOMS-Nimbus7 in order to extend the MSR2 data record backward into the 1960s.

Table 3.1: MSR2 data product – list of input data sets.

Sensor	Time period	L2 version	Comment
BUV-Nimbus4	04/1970 – 05/1977	BUV v8.6 (L2.2.01)	
TOMS-Nimbus7	11/1978 – 04/1993	TOMS v8	
TOMS-EP	08/1996 – 12/2002	TOMS v8	
SBUV-7	11/1978 – 06/1990	SBUV v8.6	
SBUV-9	02/1985 – 02/1998	SBUV v8.6	
SBUV-11	12/1988 – 03/2001	SBUV v8.6	
SBUV-14	02/1995 – 09/2006	SBUV v8.6	
SBUV-16	10/2000 – 12/2003	SBUV v8.6	
SBUV-17	07/2002 – 12/2011	SBUV v8.6	
SBUV-18	06/2005 – 12/2011	SBUV v8.6	
SBUV-19	02/2009 – 12/2011	SBUV v8.6	
GOME	06/1995 – 06/2011	GDP5 and TOGOMI v2	
SCIAMACHY	08/2002 – 04/2012	SGP v5.02W and TOSOMI v2	
OMI	10/2004 – 12/2022	OMTO3 and OMDOAO3	
GOME-2A	01/2007 – 11/2021	GDP4.6-4.8	

Sensor	Time period	L2 version	Comment
GOME-2B	05/2013 – 12/2022	GDP4.8	
GOME-2C	11/2019 – 12/2022	GDP4.8	
OMPS-NM	11/2011 – 12/2022	TO3 v2.1	
TROPOMI	05/2018 – 12/2022	RPRO/OFFL v2.1	
Dobson	01/1960 – 12/1978		Ground-based sensors

3.1.2 Resolution and coverage in space and time

Table 3.2 provides an overview of the technical specifications of the MSR2 L4 data product.

Table 3.2: MSR2 data product – sampling resolution and coverage in space and time.

Dimension	Specification	Notes
Temporal resolution	monthly	Computed from 6 hourly assimilation time steps
Temporal coverage	01/1960 – 12/2022	
Horizontal resolution	0.5° x 0.5°	
Horizontal coverage	global	
Vertical resolution	n/a	
Vertical coverage	total column	

3.1.3 Uncertainty estimates, quality indicators, and expected accuracy

The expected quality of MSR2 is summarised in Table 3.3.

Table 3.3: Expected quality of MSR2 data product.

Quantity	Specification	Notes
Accuracy : systematic component	<1%	Based on comparisons to ground-based ZSL-DOAS measurements [RD-6]
Accuracy : random component	2%	Based on comparisons to ground-based ZSL-DOAS measurements [RD-6]
Stability	0.5% / decade	Based on comparisons to ground-based ZSL-DOAS measurements [RD-6]

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: MSR2 data product – List of variables and description.

Variable	Unit	Dimension	Longname / description / comment
time	months	N_{time}	number of months since Jan 1960
latitude	degree N	N_{lat}	
longitude	degree E	N_{lon}	
total_ozone_column	DU	N_{time} x N_{lat} x N_{lon}	mean total ozone
total_ozone_column_ standard_deviation	DU	N_{time} x N_{lat} x N_{lon}	standard deviation of mean total

Table 3.5: MSR2 data product – List of metadata.

Metadata name	Comment
Authors	
Affiliation	
Email	
Date_created_by	
Ozone_field_date	
Date_format	
Number_of_longitudes	
Longitude_range	
Longitude_step	
Number_of_latitudes	
Latitude_range	
Latitude_step	
Field_Average_O3_column	
Field_Average_O3_std	
Units	
Undefined_value	
Datafile_generated_at	
Note	

3.1.5 Data volume

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

Table 3.6: MSR2 data product – Estimates of data volume.

	Month	Year	Full period
Data volume	1 MB	12 MB	800 MB

4 Tropospheric ozone

Three complementary techniques are employed to derive tropospheric ozone column data products: Convective Cloud Differential (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 (CCD and LNM). Specifications for the Optimal Estimation (i.e., ozone profile retrieval from nadir sensors) products can be found in Sect. 5, since the layer containing tropospheric ozone information can be extracted from the nadir profile products (that also cover stratosphere and upper atmosphere).

4.1 Tropical Tropospheric Ozone 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 GOME-type Tropical Tropospheric Ozone Essential Climate Variable scheme (GTTO-ECV) 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.

4.1.1 Used input data

The CCD technique relies on the availability of total ozone column and cloud data. Data from seven UV-visible nadir sensors are 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 was used to maximise consistency of the time series.

Table 4.1: GTTO-ECV 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.
GOME-2C	07/2019 – present	GODFIT v4	Extended by the C3S service.

Sensor	Time period	L2 version	Comment
TROPOMI	05/2018 – present	RPRO/OFFL V2.4.1	Extended as part of ESA's ATM-MPC. The processor uses the GODFIT v4 algorithm.

4.1.2 Resolution and coverage in space and time

Table 4.2 provides an overview of the technical specifications of the GTTO-ECV L3 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 4.2: GTTO-ECV 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).

4.1.3 Uncertainty estimates, quality indicators, and expected accuracy

The expected quality of GTTO-ECV is summarised in Table 4.3.

Table 4.3: Expected quality of GTTO-ECV data product.

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

4.1.4 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 4.4 lists the name, units, dimensions and a description of the data variables. Table 4.5 presents the included metadata.

Table 4.4: GTTO-ECV 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 4.5: GTTO-ECV 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_stratosphere	
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	

4.1.5 Data volume

An estimate of the file sizes is given in Table 4.6.

Table 4.6: GTTO-ECV data product– Estimates of data volume.

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

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

The Limb-Nadir Matching (LNM) technique combines total ozone column data from nadir sensors and stratospheric ozone profile data from limb sensors. Two complementary LNM data products will be developed: one uses OMI level-2 data as a source of total ozone (OMI-LIMB), the other uses the multi-sensor merged GTO-ECV level-3 total ozone record developed during earlier phases of CCI and extended as part of C3S operations (GTO-LIMB). The stratospheric profile information originates from the gap-free high-resolution gridded limb data product presented in Section 6.1. Each LNM product contains two tropospheric columns: one from surface to thermal tropopause, another from surface to 3 km below the thermal tropopause.

4.2.1 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 6.1. Total column data comes either from an OMI level-2 product or from the GTO-ECV level-3 merged product.

Table 4.7: OMI-LIMB and GTO-LIMB data products – list of input data sets.

Sensor / data set	Time period	Data version	Comment
OMI	2004 – present	GODFIT L2 v4	total ozone (L2)
GTO-ECV	1995 – present	GTO-ECV L3 v3.0	multi-sensor total ozone (L3)
High-resolution merged limb	2001 – present	(see Section 6.1)	ozone profile (L3)

4.2.2 Resolution and coverage in space and time

Table 4.8 provides an overview of the technical specifications of the OMI-LIMB and GTO-LIMB data products. These provide monthly mean tropospheric ozone for two partial columns since early 2000s.

Table 4.8: OMI-LIMB and GTO-LIMB data products – sampling resolution and coverage in space and time.

Dimension	Specification	Notes
Temporal resolution	monthly	
Temporal coverage	OMI-LIMB: 2004 – present; 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

4.2.3 Uncertainty estimates, quality indicators, and expected accuracy

The expected quality of OMI-LIMB and GTO-LIMB is summarised in Table 4.9.

Table 4.9: Expected quality of GTTO-ECV data product.

Quantity	Specification	Notes
Accuracy : systematic component	tbd	Pending validation
Accuracy : random component	3-9 DU (typically ~6 DU)	
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 4.10 lists the name, units, dimensions and a description of the data variables. Table 4.11 presents the included metadata.

Table 4.10: OMI-LIMB and GTO-LIMB data products – 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}	

Variable	Unit	Dimension	Longname / description / comment
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
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 4.11: OMI-LIMB and GTO-LIMB data products – 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+ (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
value_for_nodata	NaN

4.2.5 Data volume

An estimate of the file sizes is given in Table 4.12.

Table 4.12: OMI-LIMB and GTO-LIMB data products – Estimates of data volume.

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

5 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.

5.1 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. The algorithm is still being refined and the resulting prototype data will not be publicly released.

5.1.1 Used input data

Data from four UV-visible nadir sensors are considered, starting with OMI in 2004 and continuing to present with several sensors based on an evolved GOME instrument design.

Table 5.1: RAL prototype data products – list of input data sets.

Sensor	Time period	L1 version	Comment
GOME-2B	01/2013 – 12/2023	EUMETSAT L1 v6.3 and v7.0	Sampled 9-10 d per month
GOME-2C	01/2019 – 12/2023	EUMETSAT L1 v6.3 and v7.0	Sampled 9-10 d per month
OMI	10/2004 – 12/2023	NASA Collection 4	Sampled 6 d per month
S5p	05/2018 – 12/2023	ESA reprocessed v2.01	Sampled 3 d per month

5.1.2 Resolution and coverage in space and time

Table 5.7 provides an overview of the technical specifications of the RAL L2 prototype data products. 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.

Table 5.2: RAL prototype data products – sampling resolution and coverage in space and time.

Dimension	Specification	Notes
Temporal resolution	daily	
Temporal coverage	01/2013 – 12/2023	Start time depending on sensor

Dimension	Specification	Notes
Horizontal resolution	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	

5.1.3 Uncertainty estimates, quality indicators, and expected accuracy

The expected quality of RAL products is summarised in Table 5.8.

Table 5.3: Expected quality of RAL prototype data products.

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

5.1.4 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 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 5.4: RAL prototype data products – List of variables and description.

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

Variable	Unit	Dimension	Longname / description / comment
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
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

Variable	Unit	Dimension	Longname / description / comment
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
convergence_flag _uv1	1	scanline_uv1 ground_pixel_uv1	Convergence flag
convergence_flag_solar	1	ground_pixel	Convergence flag
convergence_flag_solar_uv1	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_uv1	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)

Variable	Unit	Dimension	Longname / description / comment
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
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

5.1.5 Data volume

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

Table 5.5: RAL prototype data products – Estimates of data volume.

	Month	Year	Full period
GOME-2B (9-10d/month)	1.5 GB	17 GB	183 GB
GOME-2C (9-10d/month)	1.5 GB	17 GB	72 GB
OMI (6d/month)	3.8-7.1 GB	45-85 GB	1.1 TB
S5P (3d/month)	16 GB	170 GB	720 GB

5.2 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.

5.2.1 Used input data

Data from five UV-visible nadir sensors are considered, starting with GOME in 1995 and continuing to 2021 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 5.6: 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 – 10/2021	v03.03 (01/2015 – 10/2020); v03.05 (11/2020 – 10/2021)	

5.2.2 Resolution and coverage in space and time

Table 5.7 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 5.7: GOP-ECV data product – sampling resolution and coverage in space and time.

Dimension	Specification	Notes
Temporal resolution	monthly	
Temporal coverage	07/1995 – 10/2021	
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	

5.2.3 Uncertainty estimates, quality indicators, and expected accuracy

The expected quality of GOP-ECV is summarised in Table 5.8.

Table 5.8: 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

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 5.9: 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 5.10: GOP-ECV data product – List of metadata.

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

Metadata name	Comment
sensor	
key_variables	

5.2.5 Data volume

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

Table 5.11: GOP-ECV data product – Estimates of data volume.

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

5.3 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 Level-2 O3 profile 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.

5.3.1 Used input data

The IASI L2 O3 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 5.12: 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 data	https://navigator.eumetsat.int/product/EO:EUM:DAT:METOP:IASIL1C-ALL
IASI-C	2019 – 2023	Operational IASI L1c data	https://navigator.eumetsat.int/product/EO:EUM:DAT:METOP:IASIL1C-ALL

5.3.2 Resolution and coverage in space and time

Table 5.13 provides an overview of the technical specifications of the IASI L2 data products.

Table 5.13: 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: 2008-2018; IASI-B: 2013-present; IASI-C: tbd	
Horizontal resolution	12 km circle diameter (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	

5.3.3 Uncertainty estimates, quality indicators, and expected accuracy

The expected quality of IASI level-2 data is summarised in Table 5.14.

Table 5.14: 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) are not taken into account in the total retrieval error matrix.

Quantity	Specification	Notes
Accuracy : random component	<35% along the profile	Profile: 10-35% (troposphere), 5-30% (stratosphere, usually <15%); Total columns: < 10% (usually ~3%)
Stability	Tbd	No significant bias due to instrument aging: when comparing IASI-A and IASI-B total ozone columns, the bias is generally within 0.5%.

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 5.15 lists the name, units, dimensions and a description of the data variables. Table 5.16 presents the included metadata.

Table 5.15: IASI level-2 data products – List of variables and description.

Variable	Unit	Dimension	Longname / description / comment
time	second	N_{time}	UTC observation time in seconds since 2007-01-01 00:00:00 UTC
time_string	n/a	N_{time} x $N_{chartime}$	UTC observation time as YYYYMMDDThhmmssZ
time_in_day	second	N_{time}	UTC observation time in seconds in the day
latitude	degree N	N_{time}	Latitude of ground pixel center
longitude	degree E	N_{time}	Longitude of ground pixel center
solar_zenith_angle	degrees	N_{time}	Solar zenith angle at the Earth's surface for the pixel center
satellite_zenith_angle	degrees	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

Variable	Unit	Dimension	Longname / description / comment
retrieval_quality_flag	n/a	N_{time}	Retrieval quality flag summarizing processing flags: 2 for the most reliable pixel; 1 for valuable pixels, but to use with caution; 0 for the remaining pixels that are not recommended for use
surface_altitude	m	N_{time}	Altitude of the surface
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_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. These errors are relative to the ozone partial column in each layer; they are without unit.
O3_total_column	mol m^{-2}	N_{time}	Retrieved ozone total column.
O3_total_column_error		N_{time}	Total retrieval error associated to ozone total column. This error is relative to the ozone total column; it is without unit.
O3_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

Variable	Unit	Dimension	Longname / description / comment
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 5.16: IASI level-2 data products – List of metadata.

Metadata name	Comment
Title	IASI/METOP-"X" EUMETSAT CDR ozone (O3) L2 products (profiles of partial columns and total columns)
Institution	ULB for algorithm development ; EUMETSAT for data production ; LATMOS for data extraction and formatting
Source	EUMETSAT IASI Level 2 CDR ozone (O3) release 1
History	YYYY-MM-DD HH:MM:SS (date of data extraction) - Product generated with FORLI v20151001 at EUMETSAT
References	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_"yyyymmdd"_EUMETSAT_CDR_"version".nc
Tracking_id	
Conventions	CF-1.6
Product_version	CDR Release 1 of IASI 2b - 1st extraction
Summary	IASI L2 data were reprocessed by EUMETSAT to product an 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. This dataset contains Level 2 ozone profile and total column products from IASI observations. Data reconstruction and formatting in netcdf files are processed by LATMOS.
Keywords	satellite,observation,atmosphere,ozone,O3,level 2,column,altitude,profile,pollution,IASI,Metop-A and -B
Keywords_vocabula	GCMD Science Keywords

Metadata name	Comment
Creator_name	ULB-LATMOS
Creator_type	cfr "Institution"
Contact_email	contact form at http://iasi.aeris-data.fr/contact/
Data_policy	see https://iasi.aeris-data.fr/data-use-policy/
geospatial_lat_min	
geospatial_lat_max	
geospatial_latitude_units	
geospatial_lon_min	
geospatial_lon_max	
geospatial_longitude_units	
geospatial_vertical_min	
geospatial_vertical_max	
time_coverage_start	
time_coverage_end	
standard_name_vocabulary	NetCDF Climate and Forecast (CF) Medata Convention version 73, 23 June 2020
platform	Metop-A or -B
sensor	IASI
spatial_resolution	12km at nadir

5.3.5 Data volume

An estimate of the file sizes is given in Table 5.17. 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 5.17: IASI level-2 data products – Estimates of data volume, representing a subsample of 4 days per month.

	Month	Year	Full period
Data volume (4 days per month)	~11 GB per IASI sensor	~125 GB per IASI sensor	IASI-A : ~1.8 TB; IASI-B : ~1.2 TB

5.4 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.

5.4.1 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 5.18: 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

5.4.2 Resolution and coverage in space and time

Table 5.19 provides an overview of the technical specifications of the IASI data product.

Table 5.19: 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	IASI-A: 2008-2018; IASI-B: 2013-present; IASI-C: 2019-present	
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 - 40 km	

5.4.3 Uncertainty estimates, quality indicators, and expected accuracy

The expected quality of IASI merged is summarised in Table 5.20.

Table 5.20: Expected 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%)

Quantity	Specification	Notes
Stability	Tbd	No significant bias due to instrument aging: when comparing IASI-A and IASI-B total ozone columns, the bias is generally within 0.5%.

5.4.4 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 5.21 lists the name, units, dimensions and a description of the data variables. Table 5.22 presents the included metadata.

Table 5.21: 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°
atmosphere_pressure_grid	Pascal	N_{lat} x N_{lon} x $N_{pressures}$	Mean pressures in bins corresponding to levels used to define inversion layers: 40 layers of about 1 km height between Earth's surface and 40 km
O3_partial_column_profile	mol m^{-2}	N_{lat} x N_{lon} x N_{layers}	Merged ozone partial column vertical profile retrieved in the layers defined by the levels given in the variable atmosphere_pressure_grid
O3_partial_column_error	n/a	N_{lat} x N_{lon} x N_{layers}	Vertical profile of total retrieval error associated to the merged ozone partial column vertical profile in the layers defined by the levels given in the variable atm sphere_pressure_grid. These errors are relative to the merged ozone partial column in each layer; they are without unit.
O3_total_column	mol m^{-2}	N_{lat} x N_{lon}	Merged ozone total column
O3_total_column_error		N_{lat} x N_{lon}	Total retrieval error associated to the merged ozone total column. This error is relative to the ozone total column; it is without unit.
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

Variable	Unit	Dimension	Longname / description / comment
O3_total_column_ averaging_kernel	n/a	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 5.22: 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
Source	IASI Level-2 FORLI-O3 v20191122
History	Product generated with FORLI-O3 v20191122 at ULB
creator_name	ULB-LATMOS
creator_email	
geospatial_lat_resolution	1 deg
geospatial_lon_resolution	1 deg
geospatial_lat_min	-90 deg
geospatial_lat_max	90 deg
geospatial_lon_min	-180 deg
geospatial_lon_max	180 deg
geospatial_vertical_min	0 km
geospatial_vertical_max	40 km
value_for_nodata	NaN
platform	IASI-A: 2008-2012; IASI-A and -B: 2013-2018; IASI-B and -C: 2019-present
sensor	IASI

5.4.5 Data volume

An estimate of the file sizes is given in Table 5.23.

Table 5.23: IASI merged level-3 data product– Estimates of data volume.

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

6 Limb profile

6.1 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.

6.1.1 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 **Error! Reference source not found.**.

Table 6.1: 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 v7.2	
OMPS-LP	2012 – present	USask v1.1.0	
OMPS-LP	2012 – present	IUP-UB v3.3	
SAGE III/ISS	2017 – present	NASA v5.2	
ACE-FTS	2004 – present	v4.1/4.2	

6.1.2 Resolution and coverage in space and time

Table 6.2 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 6.2: 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° x 1°	
Horizontal coverage	global	
Vertical resolution	1-2 km	
Vertical coverage	900-0.02 hPa	lower part from SILAM CTM

6.1.3 Uncertainty estimates, quality indicators, and expected accuracy

The expected quality of LIMB-HIRES is summarised in Table 6.3.

Table 6.3: 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
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

6.1.4 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 6.4 lists the name, units, dimensions and a description of the data variables. Table 6.5 presents the included metadata.

Table 6.4: 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.

Variable	Unit	Dimension	Longname / description / comment
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 6.5: 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

6.1.5 Data volume

An estimate of the file sizes is given in Table 6.6.

Table 6.6: LIMB-HIRES data product – Estimates of data volume.

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

7 References

Hurtmans, D., Coheur, P., Wespes, C., Clarisse, L., Scharf, O., Clerbaux, C., Hadji-Lazaro, J., George, M., and Turquety, S.: FORLI radiative transfer and retrieval code for IASI, J. Quant. Spectrosc. Ra., 113, 1391–1408, 2012.