Product User Guide and Specification (PUGS)

Level 3 and Level 4 ozone columns and profiles.

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History of modifications

Version	Date	Description of modification	Chapters / Sections
v1.1	11-15.2.2019	C3S_312a_Lot4 Ozone PUGS updated	Related documents; Acronyms; Scope of the document; Executive summary
	16-26.2.2019	Info on TC updated, incl. TC_OMPS and TC_MSR	1.1.1; 1.1.2; 1.1.4; 1.3.1.1; Appendix A
		Info on IASI data updated	2.1.1; Appendix B
		Info on NP updated	3.1.1; Appendix C
		Info on LP updated, incl. LMZ_SMR and LMZ_OMPS	4.1.1; 4.1.2; Appendix D
		Target requirements reformulated and completed	1.2; 2.2; 3.1.5; 4.2
	27.2.2019	Information on data access updated	5
v1.1a	12.4.2019	Modifications implemented after revision by ASSIMILA	Executive summary; 4.1.4; 4.3.1.
v1.2	16.03.2020	Modifications after revision	Contributors 1.2.2 (Table 3) 2.2.1 (Table 9) 2.4.2 3.2.1 (Table 12) 3.2.5 4.2.6 4.4.1 5 (Table 28) Appendix A (Table 29)
v2.0	25.03.2021	General update	All
v2.1	29.04.2021	Modifications implemented after revision by ASSIMILA	Related documents 3.1.2 References
V3.0	20.02.2023	General update needed for C3S2_312a_Lot2. New products from C3S2_312a_Lot2 are added. Figures are made colour blind friendly Updated instrument listings for the MSR	All
V3.1	06.06.2023	Corrections implemented after independent review	All
V3.2	28.07.2023	Minor correction on the style of the text and product table added in the section ‘List of Datasets covered by this document’	All
V3.3	31.01.2024	Includes now reprocessed datasets + a merged nadir ozone profile product.	All
V3.4	23.04.2024	Corrections implemented after independent review	All

V3.5	01.08.2024	Minor corrections implemented after additional comments from ECMWF	All

List of Datasets covered by this document.

The ozone datasets are composed of 4 main categories, which are presented in section 1 to section 4:

- L-3 and L-4 ozone total column retrieved from UV-nadir sensors. (section 1)
- L-3 ozone total and tropospheric column retrieved from IASI. (section 2)
- L-3 ozone profile retrieved from UV-nadir sensor. (section 3)
- L-3 ozone profile retrieved from limb and occultation sensors. (section 4)

A detailed overview of all ozone data products and a version history can be found in Appendix E. A summary is given in Table 1.

Table 1: Summary of the C3S ozone products. (The CDR products containing a (*) reference in the Deliverable ID column correspond to products that were generated in a previous C3S contract). The version number mentioned here is the latest version number, for more details, see Table 36 in Appendix E.

Deliverable ID	Product title	Product type (CDR, ICDR)	Version number	Delivery date
WP2-ICDR-O3-TC-v1	GOME-2B TC GOME-2C TC OMI TC OMPS TC S5P TC	ICDR ICDR ICDR ICDR ICDR	V0200 V0100 V0200 V0100 V0100	28/02/2022
(*)	GOME TC GOME-2A TC SCIA TC	CDR CDR CDR	V0100 V0100 V0100	30/04/2017
(*)	IASI-A TC / trop. Col.	CDR	V0004	30/04/2017
WP2-ICDR-O3-IASI-TCC-v1	IASI-B TC / trop. Col. IASI-C TC / trop. Col.	ICDR ICDR	V0004 V0004	28/02/2022
WP2-ICDR-O3-GTO-TC-v1	GTO merged TC	ICDR	V2000	28/02/2022
WP2-ICDR-O3-MSR-TC-v1	MSR TC	ICDR	V0025	28/02/2022
WP2-ICDR-O3-NP-v1	GOME-2B NP OMI NP	ICDR ICDR	V0009 V0007	28/02/2022
(*)	GOME-2A NP	CDR	V0007	30/04/2017

	GOME NP SCIA NP	CDR CDR	V0006 V0006	
WP2-FDDP-O3	NP_GOP-ECV	CDR	V0100	30/11/2023
WP2-ICDR-O3-LP-v1	OSIRIS LP OMPS-SASK LP OMPS-UB LP ACE LP MLS LP SABER LP SAGE-III LP Merged zonal mean LP Merged gridded LP	ICDR ICDR ICDR ICDR ICDR ICDR ICDR ICDR ICDR	V0002 V0002 V0002 V0002 V0003 V0002 V0003 V0008 V0004	28/02/2022
(*)	MIPAS LP GOMOS LP SCIA LP SAGE2 LP HALOE LP SMR LP	CDR CDR CDR CDR CDR CDR	V0002 V0001 V0001 V0001 V0001 V0001	30/04/2017

Related documents

Reference ID	Documents
D1	Wolfmüller, M. *(ed.)* and W. Som de Cerff, R. van der A, C. Lerot, D. Loyola, G. Miles, P.-F. Coheur, V. Sofieva, A. Laeng, N. Rahpoe, K. Walker, C. Roth and N. Kalb, Ozone_cci Phase-II System Specification Document (SSD), Issue 1, Revision 0, Ozone_cci_DLR_SS_01_00, 22 April 2015. https://climate.esa.int/en/projects/ozone/
D2	Wolfmüller, M. *(ed.)* and C. Lerot, D. Loyola, M. Coldewey-Egbers, K.-P. Heue, G. Miles, R. van der A, N. Rahpoe, V.Sofieva, A. Laeng, C. Roth, J. Urban, P.-F. Coheur, R. Astoreca, R. Hargreaves, V. Sofieva and M. Weber, Ozone_cci Phase-II System Verification Report (SVR), Issue 1, Revision 1, Ozone_cci_DLR_SVR_01, 30 October 2015. https://climate.esa.int/en/projects/ozone/
D3	van der A, R.J. *(ed.)* and the Ozone_cci science team, Ozone_cci Phase-II Product Specification Document (PSD), Issue 4, Revision 6, Ozone_cci_PSD_4.6, 12 November 2015. https://climate.esa.int/en/projects/ozone/
D4	Sofieva, V. *(ed.)* and R. van der A, M. Coldewey-Egbers, C. Lerot, D. Loyola, J. van Peet, R. Siddans, N. Rahpoe, K.-P. Heue and R. Astoreca, Ozone_cci Phase-II Product User Guide (PUG), Issue 1, Revision 1, Ozone_cci_PUG_01_01, 5 December 2015. https://climate.esa.int/en/projects/ozone/
D5	van Weele, M. and the Ozone_cci science team, Ozone_cci Phase-II User Requirement Document (URD), Version 3, Ozone_cci_URD_3.0, 12 April 2016. https://climate.esa.int/en/projects/ozone/
D6	Van Roozendael, M. *(ed.)* and M. Koukouli, A. Laeng, J.-C. Lambert, D. Loyola, R. Siddans, G. Miles, G. Stieler, J. Tamminen, R. van der A, M. Weber, E. Maillard, P. Coheur, C. Wespes, D. Degenstein, J. Urban, K. Walker and C. Lerot, Ozone_cci Phase-II Data Access Requirement Document (DARD), Issue 2, Revision 1, Ozone_cci_DARD_2.1, 25 May 2016. https://climate.esa.int/en/projects/ozone/

D7	Rahpoe, N., A. Laeng, G. Stiller, M. Weber *(eds)* and R. van der A, C. Adams, P. Bernath, T. von Clarmann, M. Coldewey-Egbers, D. Degenstein, A. Dudhia, R. Hargreaves, C. Lerot, D. Loyola, J. van Peet, V. Sofieva, J. Tamminen, J. Urban, M. Van Roozendael, T. Danckaert, R. Astoreca, K.-P. Heue, K. Walker and S. Tukiainen, Ozone_cci Phase-II Algorithm Theoretical Basis Document (ATBD), Version 1, Issue 3, Revision 0, Ozone_cci_ATBD_Phase2_V1_03_00, 30 May 2016. https://climate.esa.int/en/projects/ozone/
D8	Lambert, J.-C. *(ed.)* and D. Balis, A. Delcloo, F. Goutail, J. Granville, D. Hubert, A. Keppens, R. Kivi, M. Koukouli, J.-P. Pommereau, R. Stübi, T. Verhoelst, D. Loyola, R. Siddans, R. van der A, C. Clerbaux, A. Laeng, V. Sofieva and M. Weber, Ozone_cci Phase-II Product Validation and Intercomparison Report (PVIR), Issue 2, Revision 0, Ozone_cci_Phase-II_PVIR_2.0, 30 June 2016. https://climate.esa.int/en/projects/ozone/
D9	Dameris, M. (ed.) and P. Braesicke, M. Coldewey-Egbers and M. van Weele, Ozone_cci Phase-II Climate Assessment Report (CAR), 2nd draft, CAR_Ozone_CCI-phase-2_2draft, 30 June 2016. https://climate.esa.int/en/projects/ozone/
D10	Laeng, A. *(ed.)* and T. von Clarmann, G. Stiller, V. Sofieva, N. Rahpoe, D. Degenstein, K. Walker, D. Murtagh, J.-C. Lambert, T. Verhoelst, C. Lerot, C. Clerbaux, A. Boyard, K.-P. Heue, J. van Peet, R. Siddans, R. Astoreca and J. Hadji-Lazaro, Ozone_cci Phase-II Comprehensive Error Characterization Report (CECR), Version 2, Issue 1, Revision 2, Ozone_cci_KIT_CECR_02_01_02, 22 December 2016. https://climate.esa.int/en/projects/ozone/
D11	Van Roozendael, M. *(ed.)* and C3S Ozone team, C3S Ozone Target Requirements and Gap Analysis Document (TRGAD), Version 3.11, C3S_D312b_Lot2.1.0-2020(O3)_TRD-GAD_v3.11, February 19, 2021. https://cds.climate.copernicus.eu/cdsapp#!/dataset/satellite-ozone-v1?tab=doc
D12	Van Roozendael, M. *(ed.)* and the C3S Ozone team, C3S Ozone Algorithm Theoretical Basis Document (ATBD), Version 2.1, C3S_312b_Lot2.1.1.2_202102_ATBD_v2.1, April 29, 2021. https://cds.climate.copernicus.eu/cdsapp#!/dataset/satellite-ozone-v1?tab=doc

D13	Hubert, D., A. Keppens, T. Verhoelst, J. Granville and J.-C. Lambert, C3S 312b Lot2 Ozone Product Quality Assurance Document (PQAD), Version 2.1, C3S_D312b_Lot2.2.1.1_202102_PQAD_O3_v2.1, April 29, 2021. https://cds.climate.copernicus.eu/cdsapp#!/dataset/satellite-ozone-v1?tab=doc
D14	Hubert, D., A. Keppens, T. Verhoelst, J. Granville and J.-C. Lambert, C3S 312b Lot2 Product Quality Assessment Report (PQAR), version 2.0b, C3S_D312b_Lot2.2.1.2_202105_PQAR_O3_v2.0b, June 16 2021. https://cds.climate.copernicus.eu/cdsapp#!/dataset/satellite-ozone-v1?tab=doc

Acronyms

Acronym	Definition
ACE-FTS	Atmospheric Chemistry Experiment – Fourier Transform Spectrometer
ATBD	Algorithm Theoretical Basis Document
ATSR	Along Track Scanning Radiometer
BIRA-IASB	Belgian royal Institute for Space Aeronomy
C3S	Copernicus Climate Change Service (EU)
CCI	Climate Change Initiative
CDR	Climate Data Record
CDS	Climate Data Store
CF	Climate Forecast (Conventions and Metadata)
CNES	Centre National d'Études Spatiales (France)
CNR	Consiglio Nazionale delle Ricerche (Italy)
CRG	Climate Research Group
DARD	Data Access Requirements Document
DEM	Digital Elevation Model
DHF	Data Host Facility
DIAL	Differential Absorption Lidar
DLR	German Aerospace Centre
DOAS	Differential optical absorption spectroscopy
DoD	Department of Defense (USA)
DU	Dobson unit
ECMWF	European Centre for Medium-Range Weather Forecasts
ECV	Essential Climate Variable
Envisat	Environmental Satellite (ESA)
EO	Earth Observation
EOF	Empirical orthogonal function
EOS	Earth Observing System
EP	Earth Probe
ERBS	Earth Radiation Budget Satellite
ERS	European Remote-Sensing Satellite
ESA	European Space Agency
EU	European Union
EUMETSAT	European Organisation for the Exploitation of Meteorological Satellites
FMI	Finnish Meteorological Institute
FOR	Field Of Regard
FORLI	Fast Optimal/Operational Retrieval on Layers for IASI
GAW	Global Atmosphere Watch
GCOS	Global Climate Observation System
GDP	GOME Data Processor

Acronym	Definition
GMTED2010	Global Multi-resolution Terrain Elevation Data 2010
GODFIT	GOME-type direct-fitting retrieval algorithm
GOME	Global Ozone Monitoring Experiment (aboard ERS-2)
GOME-2	Global Ozone Monitoring Experiment – 2 (aboard Metop-A, Metop-B or Metop-C)
GOMOS	Global Ozone Monitoring by Occultation of Stars
GOP	GOME-type Ozone Profile
GTO	GOME-type Total Ozone
HALOE	Halogen Occultation Experiment
IAMAP	International Association of Meteorology and Atmospheric Physics
IASI	Infrared Atmospheric Sounding Interferometer
IFAC	Istituto di Fisica Applicata “Nello Carrara”
IO3C	International Ozone Commission
IPA	Independent pixel approximation
IR	Infra-Red
IRI	Infra-Red Imager
IUP	Institute of Environmental Physics, University of Bremen
ICDR	Intermediate Climate Data Record
KIT	Karlsruhe Institute of Technology
KMI-IRM	Royal Meteorological Institute of Belgium
KNMI	Royal Netherlands Meteorological Institute
LATMOS	Laboratoire Atmosphères et Observations Spatiales
LMZ	Limb monthly zonal
LP	Limb Profile
LS	Low Stratosphere
LT	Local time
LTE	Local thermodynamic equilibrium
LUT	Look-up table
Metop	Meteorological Operational Platform (EUMETSAT). Three such platforms exists: Metop-A, Metop-B and Metop-C
MIPAS	Michelson Interferometer for Passive Atmospheric Sounding
MLER	Minimum Lambertian Equivalent Reflectivity
MLS	Microwave Limb Sounder
MM	Monthly Mean
MZM	Monthly zonal mean
MMZM	Merged monthly zonal mean
MS	Multiple scattering
MSR	Multi-Sensor Reanalysis
NASA	US National Aeronautics and Space Administration
NDACC	Network for the Detection of Atmospheric Composition Change
NetCDF	Network Common Data Form (data file format)

Acronym	Definition
NKUA	National and Kapodistrian University of Athens
NOAA	US National Oceanic and Atmospheric Administration
NP	Nadir profile
NPP	Suomi National Polar-orbiting Partnership (NOAA / NASA / DoD)
O_3	Ozone
ODS	Ozone-Depleting Substance
OMI	Ozone Monitoring Instrument (aboard EOS-Aura)
OMPS	Ozone Mapping and Profiler Suite
OMPS-LP	OMPS Limb Profiler
OMPS-NM	OMPS Nadir Mapper
OSIRIS	Optical Spectrograph and InfraRed Imaging System (aboard Odin)
PCA	Principal component analysis
PSD	Product Specification Document
PUG	Product User Guide
RAL	Rutherford Appleton Laboratory
RMIB	Royal Meteorological Institute of Belgium
RMS	Root mean square
RT	Radiative transfer
SAA	Solar azimuth angle
SABER	Sounding of the Atmosphere using Broadband Emission Radiometry
SAGE	Stratospheric Aerosol and Gas Experiment
SBUV	Solar Backscatter Ultraviolet Radiometer
SCIA	SCIAMACHY
SCIAMACHY	Scanning Imaging Absorption Spectrometer for Atmospheric CHartographY (aboard Envisat)
SHADOZ	Southern Hemisphere Additional Ozonesondes programme
SMR	Sub-Millimetre Radiometer (aboard Odin)
SVD	Singular Value Decomposition
SZA	Solar Zenith Angle
TC	Total column
TEC	Technical Expertise Centre of CNES
TIMED	Thermosphere Ionosphere Mesosphere Energetics Dynamics
TIR	Thermal Infrared
TOA	Top of the atmosphere
TOMS	Total Ozone Mapping Spectrometer
TP	Tropopause
TPM	ESA Third Party Mission
UARS	Upper Atmosphere Research Satellite
UiB	Universität Bremen
UNEP	United Nations Environment Programme
UPMC	Université Pierre et Marie Curie

Acronym	Definition
UT	Upper Troposphere
UV	Ultraviolet
UV-Vis	Ultraviolet and visible light
VZA	Viewing Zenith Angle
WMO	World Meteorological Organization
WOUDC	World Ozone and Ultraviolet Radiation Data Centre

List of Tables

General definitions

Essential climate variable (ECV)

An ECV is a physical, chemical, or biological variable or a group of linked variables that critically contributes to the characterization of Earth's climate (Bojinski et al., 2014).

Climate data record (CDR)

The US National Research Council (NRC) defines a CDR as a time series of measurements of sufficient length, consistency, and continuity to determine climate variability and change (National Research Council, 2004).

Thematic climate data record (TCDR)

A thematic climate data record (TCDR) is a long time series of an essential climate variable (ECV) (Werschek, 2015*)*.

Intermediate climate data record (ICDR)

An intermediate climate data record (ICDR) is a TCDR which undergoes regular and consistent updates (Werschek, 2015), for example because it is being generated by a satellite sensor in operation.

Satellite data processing levels

The NASA Earth Observing System (EOS) distinguishes six processing levels of satellite data, ranging from Level 0 (L0) to Level 4 (L4) as follows:

L0 Unprocessed instrument data

L1A Unprocessed instrument data alongside ancillary information

L1B Data processed to sensor units (geo-located calibrated spectral radiance and solar irradiance)

L2 Derived geophysical variables (e.g., O_3) over one orbit

L3 Geophysical variables averaged in time and mapped on a global longitude/latitude horizontal grid

L4 Model output derived by assimilation of observations, or variables derived from multiple measurements (or both)

Table of Contents

Scope of the document

This document describes the data products generated as the C3S2_312a_Lot2 ozone data package delivery. The different satellite sensors involved and the time periods covered by each of them are listed in Table 35 (see appendix E) provides a complete list of the delivered products. Table 36 in appendix E gives an overview of the version history of all C3S products.

Most of the ozone data products described in this document have been developed as part of the ESA Ozone Climate Change Initiative projects (Ozone_cci and Ozone_cci+). They represent the current state-of-the-art in Europe for satellite-based ozone climate data record production, in line with the "Systematic observation requirements for satellite-based products for climate" as defined by GCOS (Global Climate Observing System) in (GCOS-107 2006): "Product A.7: Profile and total column of ozone".

Executive summary

The C3S2_312a_Lot2 Ozone Product User Guide and Specification (PUGS) Version 3.4 contains a full description of the ozone data products made available via the C3S CDS as of March 2024. It includes a description of target requirements and specifications for each product as well as details of the main variables. Each data file is a NetCDF4 binary file and contains a monthly L3 or L4 file.
The document is organized in four main sections, according to the four categories of the ozone data products (corresponding to the product definition in Table 35, Appendix E).

- Ozone total column (TC) retrieved from UV-nadir sensors (section **1**). Total integrated ozone vertical columns measured by passive remote-sensing UV spectrometry onboard of nadir sensors from GOME, GOME-2 (from Metop-A,B,C), SCIAMACHY, OMPS-NM, OMI and TROPOMI are presented. A TC merged product (TC_GTO-ECV) and a L4 ozone TC product is also present, the TC_MSR.
- Ozone total and tropospheric column retrieved from IASI (section **2**). The C3S ozone columns retrieved from observations by IASI on Metop-A,B,C include Level-3 monthly mean total and tropospheric columns are described here.
- Ozone profiles retrieved from UV-nadir sensors (section **3**). Mean ozone vertical profiles are given here, retrieved from the following UV nadir sensors: GOME, SCIAMACHY, GOME-2 (Metop-A,B) and OMI. A L3 nadir profile merged product (NP_GOP-ECV) is also presented.
- Ozone profiles retrieved from limb and occultation sensors (section 4)
- Mean ozone vertical profiles retrieved from twelve limb and occultation sensors or from a combination of such sensors are given here. The sensors are MIPAS, GOMOS, SCIAMACHY, SAGE2, SAGE-III, HALOE, SMR, OSIRIS, ACE, SABER, MLS and OMPS.

Section 5 provides additional information on data that is available on the C3S climate data store (CDS) at ECMWF. It is explained how the data can be accessed, where the data was produced and where the documentation of the data can be found.
In the appendices A, B, C, D and E, several tables are presented which give an overview of the characteristics of the C3S ozone products.

1. L-3 and L-4 ozone total column retrieved from UV-nadir sensors

The stratospheric ozone layer protects organisms and ecosystems on Earth from the harmful effects of solar ultraviolet radiation. A strong decline in ozone amounts attributable to anthropogenic emissions of ozone-depleting substances (ODSs) has been observed since the late nineteen eighties. Since 1987, the Montreal Protocol and its subsequent amendments control the production and release of these ODSs. Measurements indicate that stratospheric concentrations of key ODSs peaked in the late 1990s and have begun to decrease since the turn of the century. A key requirement is now the monitoring of the effectiveness of the Montreal Protocol, i.e., the detection of the expected onset of ozone recovery and its spatial fingerprint. To this aim, high-quality and stable long-term data sets are needed. Total integrated ozone vertical columns measured by passive remote-sensing UV spectrometry-based nadir sensors such as SBUV, TOMS, GOME, SCIAMACHY, OMPS-NM, OMI and TROPOMI provide stable data sets suitable for the required long-term trend assessment.

1.1 Product description

1.1.1 The data set

This class of ozone products includes ten climate data records (CDR) derived from nadir-viewing UV sensors. Seven of them are intermediate climate data records (ICDR), meaning that they are being regularly and consistently updated with new observations, since (some of) the associated instruments are still in operation. In all cases, the retrieved variable is the monthly average of the ozone total column.

Features common to the ten products are listed in Table 2. Features specific to one product or a subgroup of products are described in the following subsections.

Table 2: Common characteristics of the C3S ozone total column monthly means retrieved from UV-nadir sensors.

Originating satellite sensor type	Nadir-viewing UV sensor
Data class	Earth Observation Data
Algorithm description reference	C3S Ozone Algorithm Theoretical Basis Document (ATBD) D12
Geographic coverage	Global
Horizontal grid	1° longitude x 1° latitude
Temporal resolution	Monthly
Main variable physical nature and unit	Monthly mean ozone total column (molecules m^{-2})
Data format	CF-compliant NetCDF

1.1.2 Originating satellite/sensor system, temporal coverage and ICDR update

All ten products include ozone column monthly means retrieved from UV-nadir observations by one or several sensors. The temporal coverage of the data depends on the life-time of the associated satellite, or rather of the sensor on board of the satellite. Columns 2, 3 and 4 of Table 3 list the observation systems, dataset version numbers in the CDS and associated time-spans of the ten products named in Column 1. All instruments are described in the C3S Ozone ATBD D12.

Table 3: Originating system, temporal coverage, algorithm name and version, and processing level of the ten C3S data products including ozone total column monthly means from UV-nadir sensors. In the case of TC_GTO-ECV the input data are individual L3 records and the output is the merged L3 product.

Product name	Originating Satellite / Sensor System	CDS version number	Temporal coverage	L1 to L2 algorithm name and version	L2 to L3 algorithm name and version	L3 to L3 algorithm name and version	L-2 to L-4 algorithm name and version	Processing level of end product
TC_GOME	ERS-2 / GOME	0100	06.1995 - 07.2011	GODFIT	UCAS V3.1	/	/	3
TC_SCIA	Envisat / SCIAMACHY	0100	08.2002 - 04.2012					3
TC_GOME2A	Metop-A / GOME-2	0100	01.2007 - 10.2021					3
TC_GOME2B	Metop-B / GOME-2	0100	01.2013 - 10.2018					3
		0101	07.2018 - 10.2022					3
		0200	01.2013 - 04.2023					3
TC_GOME2C	Metop-C / GOME-2	0100	07.2019 – 04.2023					3
TC_OMI	Aura / OMI	0100	10.2004 - 01.2019					3
		0101	01.2017 - 10.2022					3
		0200	10.2004 - 04.2023					3
TC_S5P	S5P / TROPOMI	0100	05.2018 – 04.2023					3
TC_OMPS	SNPP / OMPS-NM	0100	01.2012 - 04.2023					3
TC_GTO-ECV	ERS-2 / GOME Envisat / SCIAMACHY AURA / OMI Metop-A / GOME-2 Metop-B / GOME-2	0100	07.1995 - 06.2017	/	/	GTO-ECV V3.0	/	3
		0200	01.2007 - 06.2018					3
		0300	01.2007 - 10.2018					3
		0400	01.2007 - 07.2019					3
		0500	01.2007 - 10.2019					3
		0600	01.2007 - 04.2020					3
		0700	01.2007 - 10.2020					3

Product name	Originating Satellite / Sensor System	CDS version number	Temporal coverage	L1 to L2 algorithm name and version	L2 to L3 algorithm name and version	L3 to L3 algorithm name and version	L-2 to L-4 algorithm name and version	Proces-sing level of end product
	ERS-2 / GOME Envisat / SCIAMACHY AURA / OMI Metop-A / GOME-2 Metop-B / GOME-2 Metop-C / GOME-2 S5P / TROPOMI	0800	01.2007 – 10.2021					3
		0900	01.2013 – 04.2022					3
		1000	01.2013 – 10.2022					3
		1100	01.2013 – 04.2023					3
		2000	07.1995- 04.2023					3
TC_MSR	ERS-2 / GOME Envisat / SCIAMACHY AURA / OMI Metop-A / GOME-2 Metop-B / GOME-2 Metop-C / GOME-2 Nimbus4 / BUV Nimbus7 / TOMS EP / TOMS SBUV series NPP / OMPS S5P / TROPOMI	0020	04.1970 - 06.1976 10.1976 - 07.1977 09.1977 - 11.1977 10.1978 - 01.2018	/	/	/	TMDAM	4
		0021	01.1979 - 12.2018					
		0022	12.2018 - 12.2020					
		0023	04.1970- 12.2018					
		0024	12.2018- 12.2021					
		0025	01.2022- 12.2022					

The update frequency and latency of the seven ICDR's are as follows.

- TC_GOME2B, TC_GOME2C, TC_OMI, TC_OMPS and TC_S5P are updated quarterly with a 4-month delay.
- TC_GTO-ECV is updated semi-annually with a 4-month delay.
- TC_MSR is updated annually with a 2-month delay.

1.1.3 Algorithm and processing level

Names and version numbers of algorithms applied within the C3S Ozone project to derive UV-nadir ozone columns are listed in Columns 5, 6, 7 and 8 of Table 3. Column 9 provides the processing level of the data included in the end products made available to the C3S data store (named in Column 1).

Algorithms to transform Level-0 into Level-1 data (radiances along the satellite swaths) are described in the ATBDs of the different instruments - see references cited in the C3S Ozone ATBD D12.

The GODFIT algorithm developed at BIRA-IASB is applied to retrieve ozone columns (Level-2) from radiances (Level-1). It is described in detail in the C3S Ozone ATBD D12 (Section 3.1.2).

The eight C3S data products that include Level-3 monthly mean ozone columns retrieved from individual sensors (see first six entries in Table 3) are generated from the corresponding Level-2 datasets by DLR using the UCAS algorithm. The algorithm applied to transpose ozone data along the satellite paths (Level-2) to ozone data on a regular longitude-latitude grid (Level-3) is described in Section 3.1.3.1 of the C3S Ozone ATBD D12.

The algorithm giving rise to the Level-3 merged GOME-type total ozone (GTO-ECV) by combination of Level-3 ozone data from GOME, GOME2, SCIAMACHY, OMI and TROPOMI is described in Section 3.1.3.2 of the C3S Ozone ATBD D12.

The multi-sensor reanalysis (MSR) producing the Level-4 TC_MSR dataset by assimilation of Level-2 ozone columns observed by a large number of UV-nadir sensors is described in Section 3.1.4 of the C3S Ozone ATBD D12 .

1.1.4 Ancillary data: auxiliary parameters used in the GODFIT algorithm

Table 4 lists static and dynamic auxiliary data needed by the retrieval algorithm GODFIT to generate the total ozone ECV.

Table 4: List of auxiliary input needs for generating the Level 2 total ozone product with the GODFIT retrieval algorithm.

Parameter	unit	Source	Comments
High-resolution solar spectrum	[molecules s^{-1} m^{-2} nm^{-1}]	Chance and Kurucz [2010]	Static
Absorption O_3 cross sections at various temperatures	[cm^2molecule sec.$^{-1}$]	Serdyuchenko et al., [2014]	Static
Ring cross-sections	---	Generated internally	Static
Surface Albedo	---	OMI-based monthly LER database (Kleipool et al. [2008])	Static Values at 335 nm are used
Surface height	m	GMTED2010 [https://www.usgs.gov/land-resources/eros/coastal-changes-and-impacts/gmted2010?qt-science_support_page_related_con=0#qt-science_support_page_related_con]	Static Degraded at instrumental resolution

Parameter	unit	Source	Comments
A-priori O_3 vertical profile shapes	DU	Total O_3-classified climatology (Labow et al., [2015]) combined with the OMI/MLS tropospheric O_3 climatology (Ziemke et al., [2011])	Static
Cloud fraction	---	Cloud product FRESCOv7/O2-02 OMI product or extracted from NASA TO3 OMPS product	Dynamic
Cloud top height/pressure	Pa	Cloud product FRESCOv7/O2-02 OMI product or extracted from NASA TO3 OMPS product	Dynamic
Temperature profiles	K	ECMWF - ERA Interim and ERA5	Dynamic Only to compute soft-calibration factors.

1.1.5 Bias corrections

1.1.5.1 Ozone column from individual sensors

No bias corrections have been applied to level-3 data from the individual sensors.

1.1.5.2 Merged UV-nadir ozone column (GTO-ECV)

Before merging the monthly mean level-3 ozone columns from the individual sensors into the GTO-ECV product bias corrections have been applied to GOME, SCIAMACHY, GOME-2A, and GOME-2B in which OMI has been used as a reference. A detailed description of this procedure can be found in Section 3.1.3.2 of the C3S Ozone ATBD D12 .

1.2 Target requirements

Table 5 lists selected dataset properties (Dataset property) together with their values as defined in the *a priori* data specification of Appendix A (Specification) and the values required by users: Target (goal) and Threshold, as presented in the C3S Ozone Target Requirements and Gap Analysis Document (TRGAD) D11. If more demanding, GCOS targets are also mentioned.

Table 5**:** Specified values of selected properties of the C3S ozone total column monthly mean retrieved from UV-nadir sensors (Column 4), with their user-required target and threshold values (Columns 2 and 3). When more demanding than the documented requirements, GCOS targets are mentioned in brackets.

Dataset property	User requirement (*)		C3S	
	Target (goal)	Threshold	Specification	Data products
Geographic coverage	Global (incl. polar night)	Global	Global	all
Horizontal resolution	20 km	100 km	1° x 1°	all
Total uncertainty (**)	2%	3%	5%	TC_GOME

Dataset property	User requirement (*)		C3S	
	Target (goal)	Threshold	Specification	Data products
			3%	TC_SCIA TC_GOME2A TC_GOME2B TC_GOME2C TC_OMI TC_OMPS TC_S5P TC_GTO-ECV
			2%	TC_MSR
Stability (**)	1% / decade	3% / decade	1% / decade	all
ICDR update frequency	Daily (GCOS: 4-hourly)	Weekly	Quarterly	TC_GOME2B TC_GOME2C TC_OMI TC_OMPS TC_S5P
			Semi-annually	TC_GTO-ECV
			Annually	TC_MSR

(*) As documented in the C3S Ozone Target Requirements and Gap Analysis Document (TRGAD)D11
(**) As defined in the C3S Ozone PQAD D13.

The gap possibly occurring between the actual value of the dataset uncertainty or stability and the corresponding specification (Appendix A) is monitored through key performance indicators (KPI) that are made available to ECMWF and to the project partners.

1.3 Data usage information

1.3.1 Data file content, format and names

1.3.1.1 Ozone column from individual UV-nadir sensors and merged ozone column (GTO-ECV)

Table 6 describes all variables contained in the NetCDF files of the products TC_GOME, TC_SCIA, TC_GOME2A, TC_GOME2B, TC_GOME2C, TC_OMI, TC_OMPS, TC_S5P, and TC_GTO-ECV.

Table 6: Dimension and description of all variables contained in the individual and merged L3 monthly mean total ozone NetCDF files. Nlat = 180 and Nlon = 360.

Variable Name	Unit	Dimension	Description
Latitude	degree	N_{lat}	Latitude of grid centre
Longitude	degree	N_{lon}	Longitude of grid centre
total_ozone_column	molecules m^{-2}	N_{lat} x N_{lon}	Mean Total Ozone Column
total_ozone_column_standard_deviation	molecules m^{-2}	N_{lat} x N_{lon}	Standard Deviation of Mean Total Ozone Column

Variable Name	Unit	Dimension	Description
total_ozone_column_standard_error	molecules m^{-2}	N_{lat} x N_{lon}	Standard Error of Mean Total Ozone Column
total_ozone_column_number_of_observations	-	N_{lat} x N_{lon}	The Number of Measurements used to derive the Mean Total Ozone

1.3.1.2 Multi-sensor reanalysis (MSR)

Table 7 describes all variables contained in the NetCDF files of the TC_MSR product.

Table 7: Dimension and description of all variables contained in the L4 merged monthly mean total ozone NetCDF files. Nlat = 361, Nlon = 720.

Variable Name	Unit	Dimension	Description
latitude	degree	N_{lat}	Latitude of grid centre
longitude	degree	N_{lon}	Longitude of grid centre
time	Days	N_{days}	number of days since 1970-01-15 00:00:00
total_ozone_column	DU	N_{days} X N_{lat} x N_{lon}	Mean Total Ozone Column in Dobson Units
total_ozone_column_standard_deviation	DU	N_{days} X N_{lat} x N_{lon}	Standard Deviation of Mean Total Ozone Column in Dobson Units

1.3.2 Quality indicators for the multi-sensor reanalysis (MSR)

The standard deviation is a useful criterion as an assessment of the data quality. If the error is more than 20 DU, it is advised not to use this data value, since there have been likely no observations for some time over this grid cell.

1.3.3 Other useful information

1.3.3.1 Ozone column from individual sensors

In order to provide representative monthly mean values that contain a sufficient number of measurements equally distributed over all days in a month, cut-off values for latitude as a function of month have been defined (see Table 8). These cut-off values are applied during the calculation of the monthly means.

GOME/ERS-2 lost its global coverage in June 2003 due to an on-board tape recorder failure. Thus, since that date coverage of TC_GOME monthly mean level-3 ozone columns is limited to the regions where the platform was in direct contact with ESA ground receiving stations.

1.3.3.2 Merged UV-nadir ozone columns (GTO-ECV)

As for the monthly mean ozone columns from individual sensors (see Section 1.3.3.1), cut-off values for latitude as a function of month have been defined (see Table 8). These cut-off values are applied during the calculation of the monthly means.

Table 8: Cut-off values for latitude as a function of month for the individual and merged UV nadir level 3 monthly mean total ozone products.

Month	Latitudes	Month	Latitudes
January	60.0° N – 90.0° S	July	90.0° N – 57.5° S
February	70.0° N – 90.0° S	August	90.0° N – 62.5° S
March	80.0° N – 80.0° S	September	82.5° N – 72.5° S
April	90.0° N – 65.0° S	October	72.5° N – 85.0° S
May	90.0° N – 60.0° S	November	65.0° N – 90.0° S
June	90.0° N – 57.5° S	December	60.0° N – 90.0° S

1.3.4 Data disclaimer

No known issues.

2. L-3 ozone total and tropospheric column retrieved from IASI

Space observation in the nadir geometry is the most efficient way to obtain global information on horizontal distribution of O_3, along with coarse information on the vertical axis. However, in contrast to total ozone, retrievals of tropospheric O_3 remain challenging since most of the O_3 is contained in the stratosphere. Although tropospheric O_3 columns were first derived from backscatter nadir UV measurements by subtracting an estimate of the stratospheric component from the measured total column (e.g., Fishman and Larsen, 1987), the recently developed thermal infrared (TIR) nadir-viewing spectrometers offer more sensitivity in the troposphere, as demonstrated by the Infrared Atmospheric Sounding Interferometer (IASI) on board Metop-A, -B and –C.

2.1 Product description

2.1.1 The data set

The C3S ozone columns retrieved from observations by IASI include Level-3 monthly mean total and tropospheric columns. The IASI product is described in Table 9. There is no IASI-A O_3 data available between April and September 2015 because of a temporary issue related to alignment in the IASI-A L1 data.

Table 9: Level 3 ozone total and tropospheric column monthly mean from IASI.

Originating satellite / sensor system	Nadir-viewing sensor IASI on board the Metop satellites – cf. C3S Ozone ATBD D12, Section 1.1.5		
Data class	Earth Observation Data		
Data product names	Total column :	TC_IASI-A TC_IASI-B TC_IASI-C	
	Tropospheric column :	06TC_IASI-A 06TC_IASI-B 06TC_IASI-C	
Algorithm name and version number	L1 to L2:	FORLI-O3 v20151001 from Jan. 2008 till present	
	L2 to L3:	V0001, v0002, v0003, v0004 (reprocessing version)	
Algorithm description reference	C3S Ozone Algorithm Theoretical Basis Document (ATBD) D12		
Processing level	3		
Geographic coverage	Global		
Horizontal grid	1° longitude x 1° latitude		
Temporal coverage	TC_IASI-A & 06TC_IASI-A	*CDS version 0001 :*	10.2007 - 03.2015 10.2015 - 01.2020
		CDS version 0002 :	02.2020 - 07.2020
		CDS version 0003 :	12.2019 - 08.2021
		CDS version 0004 :	10.2007- 08.2021
	TC_IASI-B & 06TC_IASI-B	*CDS version 0001 :*	05.2013 - 01.2020
		CDS version 0002 :	02.2020 - 07.2020
		CDS version 0003 :	12.2019 - 07.2023

		CDS version 0004 :	03.2013 – 07.2023
	TC_IASI-C & 06TC_IASI-C	*CDS version 0001 :*	10.2019 – 11.2019
		CDS version 0003 :	12.2019 - 07.2023
		CDS version 0004 :	10.2019 – 07.2023
Temporal resolution	Monthly		
Update frequency	Quarterly		
Update delay	1 month		
The acquisition local time (hour)	LT09 or LT21		
Main variable physical nature and unit	TC_IASI-A TC_IASI-B TC_IASI-C	Monthly mean ozone total column (molecules.m^{-2})	
	06TC_IASI-A 06TC_IASI-B 06TC_IASI-C	Monthly mean ozone tropospheric column (molecules.m^{-2}) (between the ground and the altitude of 6 km)	
Data format	CF-compliant NetCDF		
Comment	There is no IASI-A O3 data between April and September 2015 because of a temporary issue related to an alignment issue in the IASI-A L1 data.		

2.1.2 Ancillary data

Ancillary data required to derive Level 2 data from the Level 1 datasets are described in Section 2.2.6 of the C3S Ozone ATBD D12.

No ancillary data are required for the generation of the L3 products.

2.1.3 Bias corrections

No bias correction is applied to the Level 3 products.

2.2 Target requirements

Table 10 lists selected dataset properties (Column 1) together with their values as set in the *a priori* data specification of Appendix B (Column 4) and the values required by users (Columns 2 and 3), as collected in the C3S Ozone Target Requirements and Gap Analysis Document (TRGAD)D11. If more demanding, GCOS targets are also mentioned.

Table 10: Specified values of selected properties of the C3S ozone total and tropospheric column monthly means retrieved from IASI (Column 4) with their user-required target and threshold values (Columns 2 and 3). When more demanding than the documented requirements, GCOS targets are mentioned in brackets.

Dataset property	**User requirement (*)**		**C3S**	
	Target (goal)	**Threshold**	**Specification (0)**	**Data products**
Geographic coverage	Global (incl. polar night)	Global	Global	all

Dataset property	User requirement (*)		C3S	
	Target (goal)	Threshold	Specification (0)	Data products
Horizontal resolution	20 km	100 km	1° x 1°	TC_IASI-A TC_IASI-B TC_IASI-C
		200 km	1° x 1°	06TC_IASI-A 06TC_IASI-B 06TC_IASI-C
Total uncertainty (**)	2%	3%	3%	TC_IASI-A TC_IASI-B TC_IASI-C
	8%	16%	30%	06TC_IASI-A 06TC_IASI-B 06TC_IASI-C
Stability (**)	1% / decade	3% / decade	1% / decade	TC_IASI-A
			3% / decade	TC_IASI-B TC_IASI-C
			20% / decade	06TC_IASI-A 06TC_IASI-B 06TC_IASI-C
Update frequency	Daily (GCOS: 4-hourly)	Weekly	Quarterly	all

(*) As documented in the C3S Ozone Target Requirements and Gap Analysis Document (TRGAD) D11
(**) As defined in the C3S Ozone PQAD D13.

The gap possibly occurring between the actual value of the dataset uncertainty or stability and the corresponding specification (0) is monitored through key performance indicators (KPI) that are made available to ECMWF and to the project partners.

2.3 Data usage information

2.3.1 Data file content, format and names

Common coordinates in all NetCDF output files are latitude and longitude. Missing values in the dataset are indicated with the '-999.' values.

The field 'time' is not given because monthly files are provided. The fields 'latitude' and 'longitude' give the latitude and longitude of the L3 grid cell centres. Latitude varies between -90 and +90 and longitude between -180 and +180.

The variables recorded in the NetCDF datasets are given in Table 11.

Which are the total column and its associated error (both in molecules/m^2) and the tropospheric column (defined as the column between the surface and the altitude of 6 km) and their associated errors (both in molecules/m^2) and the number of observations used for the calculation of the L3.

The daytime and night-time data are recorded in separate files.

The full list of variables in the NetCDF files can be found in Table 11.

Table 11: Dimension and description of the variables contained in the current L3 ozone NetCDF files. N_{lat} and N_{lon} represent the number of latitude and longitude points, respectively.

Variable Name	Precision and dimension	Unit	Description
Latitude	float, N_{lat}	degree	latitude, from -90 (south) to +90 (north) given at gridcell centres
Longitude	float, N_{lon}	degree	longitude, from -180 (west) to +180 (east) given at gridcell centres
total_ozone_column	float, N_{lat} x N_{lon}	molecules m^{-2}	weighted average of the total ozone columns
total_ozone_column_error	float, N_{lat} x N_{lon}	molecules m^{-2}	uncertainty in the weighted average of the total ozone columns
surface_6km_ozone_column	float, N_{lat} x N_{lon}	molecules m^{-2}	weighted average of the surface 6km ozone columns
surface_6km_ozone_column_error	float, N_{lat} x N_{lon}	molecules m^{-2}	error in the weighted average of the surface 6km ozone columns
number_of_observations	float, N_{lat} x N_{lon}	No unit	number of observations used for calculating the L3

2.3.2 Data disclaimer

Note that a drift was found in the L2 tropospheric O3 column (Boynard et al., 2018), which could lead to a significant drift in the L3 0-6km column product. This will be addressed in a future data release. The IASI L3 0-6km column product should not yet be considered of climate quality. IASI/Metop-A started drifting in September 2019, the IASI/Metop-A data for the period January 2020 – August 2021 should not be considered of climate quality. Please use IASI/Metop-B instead.

3. L-3 ozone profile retrieved from UV-nadir sensors

The total atmospheric column of ozone is routinely measured with high accuracy by UV nadir-viewing sensors (e.g. BUV, SBUV, TOMS, SBUV-2, GOME, SCIAMACHY, OMI and GOME-2). From the same type of instruments, ozone profiles have also been produced based on the exploitation of the strongly variable ozone absorption around the ozone cut-off spectral region (280-320 nm). Although retrieving tropospheric ozone presents a significant challenge in the UV (like in the TIR spectral range), tropospheric columns can be directly derived from temperature-dependent spectral structures in the Huggins bands (320–345 nm). Recently, significant effort has been devoted within the ESA CCI and CCI+ programmes to build harmonised ozone data sets from the European nadir UV spectral instruments GOME, SCIAMACHY, OMI and GOME-2. Level-3 products generated in this portfolio are based on level-2 data sets produced using a common level-2 algorithm baseline developed at RAL.

3.1 Product description

3.1.1 The dataset

This category of C3S ozone products includes Level-3 monthly mean ozone vertical profiles retrieved from five UV nadir sensors and a merged Level-3 monthly mean vertical profile. Features common to the six products are listed in Table 12. Product-specific features are described in Section 3.1.2.

Table 12: Level 3 ozone profile monthly mean from UV-nadir sensors.

Originating sensor type	Nadir-viewing UV sensor
Data class	Earth Observation Data
Algorithm description reference	C3S Ozone Algorithm Theoretical Basis Document (ATBD) D12
Processing level	3
Geographic coverage	Global
Horizontal grid	1° longitude x 1° latitude (5° longitude x 5° latitude for merged product)
Temporal resolution	Monthly
Main variable physical nature and unit	Monthly mean ozone molecular number density (cm^{-3}) Monthly mean ozone volume mixing ratio (ppmv) Monthly mean ozone partial column (molecules m^{-2})
Data format	CF-compliant NetCDF
Vertical coordinate	pressure
Vertical coverage	surface to TOA
Vertical resolution	levels at surface and at 450, 170, 100, 50, 30, 20, 10, 5, 3, 2, 1, 0.5, 0.3, 0.17, 0.1, 0.05, 0.03, 0.017 and 0.01 hPa (i.e. the L2 retrieval levels)

3.1.2 Originating satellite/sensor system, temporal coverage and ICDR update

Each of the five products includes ozone profile monthly means retrieved from UV-nadir observations by one sensor. In addition a merged product is provided. The temporal coverage of the data depends on the life-time of the associated satellite / sensor. Columns 2, 3 and 4 of Table 13 list the observation systems, dataset version numbers in the CDS and associated time-spans of the six products named in Column 1. All instruments are described in the C3S Ozone ATBD D12.

Table 13: Originating system and temporal coverage of the five C3S data products including ozone vertical profile monthly means from UV-nadir sensors. In case of NP_GOP-ECV the input data are individual L3 records and the output is the merged L3 product.

Product name	Originating Satellite / Sensor System	C3S CDS version number	Temporal coverage
NP_GOME	ERS-2/ GOME	0004	07.1995 - 05.2011
		0005	06.1995 - 06.2011
		0006	06.1995 - 06.2011
NP_SCIA	Envisat / SCIAMACHY	0004	08.2002 - 02.2011
		0005	08.2002 - 04.2012
		0006	08.2002 - 04.2012
NP_GOME2A	Metop-A / GOME-2	0004	04.2007 - 06.2013
		0005	01.2007 - 12.2017
		0006	01.2007 - 08.2019
		0007	09.2019 - 10.2020
NP_GOME2B	Metop-B / GOME-2	0005	05.2013 - 12.2017
		0006	04.2013 - 12.2017
		0007	06.2014-11.2020
		0008	11.2020-10.2021
		0009	07.2021-06.2023
NP_OMI	Aura / OMI	0004	10.2004 - 04.2012 06.2012 - 12.2015
		0005	01.2016 - 12.2017
		0006	10.2004 - 08.2019
		0007	09.2019 - 10.2021
NP_GOP-ECV	ERS-2/ GOME Envisat / SCIAMACHY Metop-A / GOME-2 Metop-B / GOME-2 Aura / OMI	0100	07.1995 – 10.2021

Two of the three ICDR in Table 13 (NP_GOME2A and NP_OMI) have been updated annually with a 4-month delay.

3.1.3 Ancillary data

Ancillary data required to derive Level 2 data from the Level 1 datasets are described in Section 2.2 of the C3S Ozone ATBD D12.

No ancillary data are required for the generation of the L3 products from the individual sensors. For the generation of the merged product NP_GOP-ECV the merged total column product TC_GTO-ECV (see Sec. 1) is needed.

3.1.4 Bias corrections

No bias correction is applied to the Level 3 products from the individual sensors. For the generation of the merged product NP_GOP-ECV bias corrections and altitude-dependent scaling is applied as described in Section 3.3.2 of the C3S Ozone ATBD D12.

3.1.5 Filters on Level 2 profiles

Other than a normal range of sanity checks on the data, Table 14 lists the specific filters that were applied for Level-3 version 0007.

Table 14: Filters applied for the L3 ozone profile dataset.

Variable	Filter
Effective Cloud Fraction(*)	-1 <= Effective Cloud Fraction < 1
Convergence(**)	True
Total ozone column	o3_tc < 1000
Cost and 'achi'(**)	GOME-2b: Cost <= 400. Other instruments: Cost <= 200. and achi == 1
GOME-2B anomaly	Scan pixels 0 -- 7 are not used
GOME-2b restrictions on total ozone column	GOME-2b, between January and May (both inclusive), o3_tc / Cos (VZA)) <= 500
GOME-2 Swath width	GOME-2a: wide swath before 2013-07-15T15:14:15.000, narrow swath afterwards (excluding nadir static or small swath modes). GOME-2b: wide swath
OMI row anomaly	only use across-track scan index 5,7,9,11,13,15,19,21,43,45,47,49,51

(*) Effective cloud fraction (ECF) here combines impact of cloud height and fraction by ECF=cloudf * Z*(cloudp)/5. Where Z* is approximate cloud height (km) from cloudp' based on scale-height, as given Eq.29 in section 3.3.1.4 of the C3S Ozone ATBD D12. Cloud pressure >1000hPa can produce -ve Z*. For a focus on tropospheric ozone, removing ECF>0.2 gives a good compromise of quality and data lost.
(**) Convergence is defined as when cost changes by <1. See section 3.3.1.4 of the C3S Ozone ATBD D12.
(***) 'achi' flag to indicate if chi-squared test passed. 1=success.

3.2 Target requirements

Table 15**Fehler! Verweisquelle konnte nicht gefunden werden.** lists selected dataset properties (Column 1), their values as set in the *a priori* data specification of appendix C (Column 5) and the corresponding values required by users (Columns 3 and 4), as a function of the atmospheric region (Column 2) and as collected in the C3S Ozone Target Requirements and Gap Analysis Document (TRGAD)D11. If more demanding, GCOS targets are also mentioned.

Table 15: Specified values of selected properties of the C3S ozone vertical profile monthly mean retrieved from UV-nadir sensors (Column 5) with their user-required target and threshold values (Columns 3 and 4) as a function of the atmospheric layer (Column 2). M = mesosphere; US = upper stratosphere; MS = middle stratosphere; LS = lower stratosphere; T = troposphere. When more demanding than the documented requirements, GCOS targets are mentioned in brackets.

Dataset property	**User requirement (*)**			**C3S**	
	Altitude region	**Target (goal)**	**Threshold**	**Specification (0)**	**Data products**
Geographic coverage		Global (incl. polar night)	Global	Global	all
Horizontal resolution	US/M	200 km (GCOS: 20 km)	400 km (GCOS: 50 km)	1° x 1°	all
	LS/MS	100 km (GCOS: 20 km)	200 km (GCOS: 50 km)		
	T	20 km	200 km		
Vertical resolution	US/M	6 km (GCOS: 3 km)	Partial column	levels at surface and at 450, 170, 100, 50, 30, 20, 10, 5, 3, 2, 1, 0.5, 0.3, 0.17, 0.1, 0.05, 0.03, 0.017 and 0.01 hPa	all
	LS/MS	6 km (GCOS: 1 km)	Partial column (GCOS: 2 km)		
	T	6 km (GCOS: 5 km)	Partial column		
Total uncertainty above TP (**)	US/M	4%	8%	20%	all
	MS	4% or 50 ppbv	8% or 100 ppbv		
	LS	8% or 50 ppbv	16% or 100 ppbv		
Total uncertainty below TP (**)	T	8%	16%	30%	all
Stability (**)		1% / decade	3% / decade	3% / decade	NP_GOME NP_OMI
				20% / decade	NP_SCIA NP_GOME2A NP_GOME2B
ICDR update frequency	US/M	Daily	Weekly	Annually	NP_GOME2A NP_GOME2B NP_OMI
	T/LS/MS	Daily (GCOS: 4h)	Weekly		

(*) As documented in the C3S Ozone Target Requirements and Gap Analysis Document (TRGAD) D11
(**) As defined in the C3S Ozone PQAD D13

The gap possibly occurring between the actual value of the dataset uncertainty or stability and the corresponding specification (0) is monitored through key performance indicators (KPI) that are made available to ECMWF and project partners.

3.3 Data usage information

3.3.1 Data file content, format and names

Common variables for all NetCDF output files are time, latitude, longitude, surface_pressure and pressure. Missing values in the dataset are indicated with the IEEE 'NaN' values.

Time is given in seconds since some reference time. Since the L3 fields are monthly averages, the time is equal to the reference time, which has been set to the first day of the month. The lat and lon fields give the latitude and longitude of the L3 grid cell centres. Latitude varies between -90 and +90 and longitude between -180 and +180.

The surface pressure and air pressure fields are given in hPa and to obtain the full 3D pressure field, one should extend the surface pressure field in the third dimension with the air pressure field. The first entry from the air pressure field should not be used, since it is only a dummy entry for the surface pressure.

The partial column datasets have been calculated for the layers between the number density levels. The full list with NetCDF variables can be found in Table 16.

Table 16: The variables in the NetCDF files containing ozone nadir profiles from the individual sensors. N_{time}, N_{layer}, N_p, N_{lat} and N_{lon} are number of time, layers, pressures levels, and latitude and longitude zones, respectively.

Parameter and unit	Dimension and precision	Description
Lon(degree East)	float, $N_{lon}\times 1$	Longitude, from -180 (west) to +180 (east) given at grid cell centres. NetCDF dimension
Lat(degree North)	float, $N_{lat}\times 1$	Latitude, from -90 (south) to +90 (north) given at grid cell centres. NetCDF dimension
Layers	integer, $N_{layer}\times 1$	Layer number, starting at 1. NetCDF dimension.
air pressure (hPa)	float, $N_p\times 1$	Air pressure at layer boundaries, replace the first element from this array with the corresponding surface pressure element. NetCDF dimension.
Time	integer, $N_{time}\times 1$	Seconds since reference time, usually the start of the month. NetCDF dimension.
surface_pressure	float, $N_{time}\times N_{lat}\times N_{lon}$	pressure at the bottom of the atmosphere
ozone partial column (molecules/m^{-2})	float, $N_{time}\times N_{layer}\times N_{lat}\times N_{lon}$	weighted average of the partial ozone columns (molecules/m2 per layer)
ozone partial column standard error (molecules/m^{-2})	float $N_{time}\times N_{layer}\times N_{lat}\times N_{lon}$	error in the weighted average of the partial ozone columns (molecules/m2 per layer)
total ozone column (molecules/m^{-2})	float, $N_{time}\times N_{lat}\times N_{lon}$	total column: vertically integrated ozone partial column dataset

Parameter and unit	Dimension and precision	Description
total ozone column standard error (molecules/m^{-2})	float, $N_{time}\times N_{lat}\times N_{lon}$	total column error: quadratically added ozone partial column standard error
ozone mixing ratio(ppmv)	float $N_{time}\times N_p\times N_{lat}\times N_{lon}$	weighted average of the volume mixing ratio
ozone mixing ratio standard error(ppmv)	float, $N_{time}\times N_p\times N_{lat}\times N_{lon}$	error in the weighted average of the volume mixing ratio
ozone concentration (molecules/m^{-3})	float $N_{time}\times N_p\times N_{lat}\times N_{lon}$	weighted average of the ozone concentration
ozone concentration standard error (molecules/m^{-3})	float $N_{time}\times N_p\times N_{lat}\times N_{lon}$	error in the weighted average of the ozone concentration

Table 17: The variables in the NetCDF files containing merged ozone nadir profiles. N_{time}, N_{layer}, N_p, N_{lat} and N_{lon} are number of time, layers, pressures levels, latitude, and longitude zones, respectively.

Parameter and unit	Dimension and precision	Description
longitude (degree East)	float, $N_{lon}\times 1$	Longitude, from -180 (west) to +180 (east) given at grid cell centers. NetCDF dimension
latitude (degree North)	float, $N_{lat}\times 1$	Latitude, from -90 (south) to +90 (north) given at grid cell centers. NetCDF dimension
pressure (hPa)	float, $N_p\times 1$	Air pressure at layer boundaries. NetCDF dimension.
ozone partial column (DU)	float, $N_{time}\times N_{layer}\times N_{lat}\times N_{lon}$	partial ozone columns (DU)
ozone partial column uncertainty (DU)	float $N_{time}\times N_{layer}\times N_{lat}\times N_{lon}$	Uncertainty of the partial ozone columns (DU)
total ozone column (DU)	float, $N_{time}\times N_{lat}\times N_{lon}$	total column: vertically integrated ozone partial column dataset

3.3.2 Data disclaimer

No known issues.

4. L-3 ozone profile retrieved from limb and occultation sensors

High-quality vertically-resolved satellite datasets are essential to assess the fate of atmospheric ozone and better understand its link with anthropogenic activities. For reliable estimates of ozone trends, long-term data records are needed in order to separate natural ozone variability (e.g. due to solar activity) and trends of anthropogenic origin. The data records presented here combine a large number of high-quality limb and occultation sensors covering a time-period suitable for trend evaluation. Ozone profile data are provided on an altitude grid or on a pressure grid depending on the native coordinate of the instrument. This ensures optimal accuracy and stability from all sensors. Ancillary information is provided with the data products to allow conversion from pressure to altitude when necessary. Merged data sets are also generated using de-seasonalised anomalies computed from each individual dataset. The main advantage of this approach is that biases due to different sampling patterns (including the difference in local time) and instrumental biases are automatically removed, which makes these data ideal for long-term analysis.

4.1 Product description

4.1.1 The dataset

This set of ozone products consists of fifteen C3S products that includes Level-3 monthly mean ozone vertical profiles retrieved from eleven limb and occultation sensors or from a combination of such sensors. Features common to the fifteen products are listed in Table 18. Product-specific features are described in Sections 4.1.2, 4.1.3 and 4.1.4.

Table 18: Level 3 ozone profile monthly mean from limb and occultation sensors.

Originating sensor type	Limb / occultation sensor
Data class	Earth Observation Data
Algorithm description reference	C3S Ozone Algorithm Theoretical Basis Document (ATBD) D12
Processing level	3
Geographic coverage	Global
Temporal resolution	Monthly
Main variable physical nature and unit	Monthly mean ozone volume mixing ratio (ppmv) (for data provided at pressure levels) Monthly mean ozone molecular concentration (molecules.m^{-3}) (for data provided on altitude levels)
Data format	CF-compliant NetCDF

4.1.2 Originating system, temporal coverage and ICDR update

The fifteen products include ozone profile monthly means retrieved from observations by one or several limb or occultation sensors. The temporal coverage of the data depends on the life-time of the associated satellite or of the sensor on board the satellite. Columns 2, 3 and 4 of Table 19 lists the

observation systems, the dataset version numbers in the CDS and the associated time-spans of the fifteen products named in Column 1. All instruments are described in the C3S Ozone ATBD D12

Table 19: Originating system and temporal coverage of the thirteen C3S data products providing ozone profile monthly means from limb or occultation sensors. Instruments with names preceded with a (*) are used to derive the additional LMZ_MERGED product. Instruments with names preceded with (**) are used to derive the two additional LMZ_MERGED and LP_MERGED products.

Product name	Originating Satellite / Sensor System	CDS version number	Temporal coverage
LMZ_MIPAS	(**) Envisat / MIPAS	0001 0002	07.2002 - 03.2004 01.2005 - 08.2005 12.2005 - 01.2006 03.2006 05.2006 - 04.2012
LMZ_GOMOS	(**) Envisat / GOMOS	0001	08.2002 - 01.2005 07.2005 - 10.2011 12.2011
LMZ_SCIA	(**) Envisat / SCIAMACHY	0001	08.2002 - 03.2012
LMZ_SAGE2	(*) ERBS / SAGE-2	0001	10.1984 - 07.2000 11.2000 - 08.2005
LMZ_HALOE	UARS / HALOE	0001	10.1991 - 09.2005
LMZ_SMR	Odin / SMR	0001	07.2001 - 08.2001 10.2001 - 08.2014
LMZ_OSIRIS	(**) Odin / OSIRIS	0001	11.2001 - 05.2018 07.2018 - 05.2019 07.2019 - 05.2020 07.2020 - 12.2020
		0002	11.2001 - 05.2018 07.2018 - 05.2019 07.2019 - 05.2020 07.2020 - 05.2021 07.2021 - 12.2022
LMZ_ACE	(*) SciSat / ACE-FTS	0001	02.2004 - 05.2011 07.2011 - 09.2011 01.2012 - 02.2012 04.2012 - 12.2020
		0002	02.2004 – 12.2022
LMZ_SABER	TIMED / SABER	0001	01.2002 - 04.2002 06.2002 - 10.2002 12.2002 - 10.2003 12.2003 - 02.2005 04.2005 - 08.2007 10.2007 - 08.2011 10.2011 - 07.2019

Product name	Originating Satellite / Sensor System	CDS version number	Temporal coverage
		0002	01.2002 - 04.2002 06.2002 - 10.2002 12.2002 - 10.2003 12.2003 - 02.2005 04.2005 - 08.2007 10.2007 - 08.2011 10.2011 - 12.2022
LMZ_MLS	Aura / MLS	0001	08.2004 - 11.2004 01.2005 - 07.2019
		0002	08.2004 - 11.2004 01.2005 - 11.2020
		0003	08.2004 - 12.2022
LMZ_OMPS-SASK	SUOMI NPP /OMPS-LP(**)	0002	02.2012 - 11.2013 01.2014 - 12.2022
LMZ_OMPS-UB	SUOMI NPP /OMPS-LP(*)	0001	02.2012 - 11.2013 01.2014 - 12.2021
		0002	02.2012 - 11.2013 01.2014 - 12.2022
LMZ_SAGE-III	ISS/SAGE-III	0001	06.2017 - 12.2022
LMZ_MERGED	Above systems marked with (*) and (**)	0001	10.1984 - 02.2017
		0002	10.1984 - 01.2018
		0003	10.1984 - 12.2018
		0004	01.2018 - 12.2019
		0005	10.1984 - 12.2019
		0006	10.1984 - 12.2020
		0007	10.1984 - 12.2021
		0008	10.1984 - 12.2022
LP_MERGED	Above systems marked with (**)	0001	11.2001 - 12.2019
		0002	11.2001 - 12.2020
		0003	11.2001 - 12.2021
		0004	11.2001 - 12.2022

The nine ICDR cited in Table 19 (last 9 lines) are updated annually with a 3-month delay.

Note that although the Odin data set is available from November 2001 until present, the validation activity performed in the framework of the Ozone_cci project identified corrupted data in the SMR record after 2010. The reprocessing of the whole SMR mission is ongoing. The re-inclusion of the LMZ_SMR dataset in the ICDR group and its regular update may therefore resume in the future.

4.1.3 Type of average, horizontal resolution and retrieval algorithm

As mentioned in Section 4.1.1 (Table 18), in all products, the main variable is the monthly mean of the ozone volume mixing ratio expressed in ppmv (on pressure levels) or of the ozone molecular concentration in molecules/cm^3 (on altitude levels).

In the fourteen "LMZ" data products, this mixing ratio (resp. concentration) is averaged over 10°-width latitude bands, or "zones". In the "LP" product, it is "gridded", i.e. averaged over 10° latitude x 20° longitude horizontal cells (Table 20).

Table 20: Type of average, horizontal resolution and retrieval algorithms of the C3S ozone profile monthly means from limb and occultation sensors.

Product name	Type of average [1]	Horizontal resolution	L2 profile harmonisation algorithm name and version	L2 to L3 algorithm name and version
LMZ_MIPAS	MZM	10° latitude zones	HARMOZ_ALT	LP-MZM-HARMOZ v1
LMZ_GOMOS	MZM	10° latitude zones	HARMOZ_ALT	LP-MZM-HARMOZ v1
LMZ_SCIA	MZM	10° latitude zones	HARMOZ_ALT	LP-MZM-HARMOZ v1
LMZ_SAGE2	MZM	10° latitude zones	HARMOZ_ALT	LP-MZM-HARMOZ v1
LMZ_HALOE	MZM	10° latitude zones	HARMOZ_PRS	LP-MZM-HARMOZ v1
LMZ_SMR	MZM	10° latitude zones	HARMOZ_PRS	LP-MZM-HARMOZ v1
LMZ_OSIRIS	MZM	10° latitude zones	HARMOZ_ALT	LP-MZM-HARMOZ v1
LMZ_ACE	MZM	10° latitude zones	HARMOZ_ALT	LP-MZM-HARMOZ v1
LMZ_SABER	MZM	10° latitude zones	HARMOZ_PRS	LP-MZM-HARMOZ v1
LMZ_MLS	MZM	10° latitude zones	HARMOZ_PRS	LP-MZM-HARMOZ v1
LMZ_OMPS-SASK	MZM	10° latitude zones	HARMOZ_ALT	LP-MZM-HARMOZ v1
LMZ_OMPS-UB	MZM	10° latitude zones	HARMOZ_ALT	LP-MZM-HARMOZ v1
LMZ_SAGE-III	MZM	10° latitude zones	HARMOZ_ALT	LP-MZM-HARMOZ v1
LMZ_MERGED	MMZM	10° latitude zones	HARMOZ_ALT	LP-MMZM v2
LP_MERGED	MM	10° latitude x 20° longitude	HARMOZ_ALT	LP-LATLON_merged v2

As seen in Section 4.1.2 (Table 19), thirteen products include data retrieved from one single sensor. The other two products combine data from a number of selected instruments, to provide zonally averaged profiles (LMZ_MERGED) or gridded profiles (LP_MERGED). For each of these last two products, concentrations and concentration anomalies are provided as two separate datasets (in separate files).

The algorithms applied to derive the end products are named in Columns 4 and 5 of Table 20. They consist in harmonising the Level-2 profiles (HARMOZ), merging them together and preserving some longitudinally resolved structure. They are described in the C3S Ozone ATBD D12.

4.1.4 Vertical coordinate

Columns 2, 3 and 4 of Table 21 provide information on the nature of the vertical coordinate, its range and resolution or number of levels for each of the "LMZ" and "LP" products.

[1] MM = Monthly mean. MZM = Monthly zonal mean. MMZM = Merged monthly zonal mean.

Table 21: Vertical domain of definition of the C3S ozone vertical profile monthly means from limb and occultation sensors. The vertical resolution indicated in the table is the vertical spacing (in km) between successive levels (approximate when the vertical coordinate is the pressure).

Product name	Vertical coordinate	Vertical coverage	Vertical resolution
LMZ_MIPAS	Altitude	6-70 km	1 km
LMZ_GOMOS	Altitude	10-105 km	1 km
LMZ_SCIA	Altitude	5-65 km	1 km
LMZ_SAGE2	Altitude	5-65 km	1 km
LMZ_HALOE	Pressure	500 - 0.02 hPa	1-3 km
LMZ_SMR	Altitude	15-65 km	1 km
LMZ_OSIRIS	Altitude	10-59 km	1 km
LMZ_ACE	Altitude	6-94 km	1 km
LMZ_SABER	Pressure	50-0.1 hPa	1-3 km
LMZ_MLS	Pressure	500 – 0.02 hPa	1-3 km
LMZ_OMPS-UB	Altitude	7-58 km	1 km
LMZ_OMPS-SASK	Altitude	7-58 km	1 km
LMZ_SAGE-III	Altitude	5-65 km	1 km
LMZ_MERGED	Altitude	10-50 km	1 km
LP_MERGED	Altitude	10-50 km	1 km

For climate studies, it is preferable to use only the information provided in the dataset (and avoid, as much as possible, using the data from models and reanalyses). For a majority of limb and occultation instruments (SAGE II, SAGE III, GOMOS, OSIRIS, SCIAMACHY, SMR, ACE-FTS, MIPAS, OMPS), ozone concentration profiles are retrieved on an altitude grid. MLS, HALOE and SABER provide mixing ratios on a pressure grid. Therefore, the monthly zonal means have the same “native” representation as original ozone profiles: ozone molecular concentration (molecules.m^{-3}) on altitude grid or ozone mixing ratio on pressure grid (Table 21). The molecular concentration values are also provided in pressure-gridded files. These data also include additional average parameters: mean temperature, pressure/altitude profiles are provided in all files.

The merged ozone profiles are ozone concentrations on an altitude grid. Concentration anomalies are also provided in separate files. To avoid ozone diurnal variations, merged ozone datasets cover the stratospheric altitude range from 10 to 50 km.

4.1.5 Ancillary data

The limb and occultation instruments use the minimum a priori information in retrievals. If the temperature profiles are not retrieved (limb-scattering and UV-VIS occultation instruments), the meteorological model/reanalysis data are used for ray tracing and computing refractive effects. However, this has a rather small impact on ozone profiles in the stratosphere (< 1 %). All European instruments use ECMWF air density and temperature fields for these computations, while SAGE II uses MERRA reanalysis data.

In addition, ozone cross-sections are used in ozone retrievals. More details on ancillary data used in retrievals from limb and occultation instruments are provided in D12.

4.1.6 Bias corrections

In the merged dataset, the biases between instruments are eliminated using deseasonalised anomalies. The profiles of merged deseasonalised anomalies can be directly used for assessment of ozone trends. For the merged monthly zonal mean dataset (LMZ_MERGED), the data before 2001 are from SAGE II solely. Therefore, the absolute ozone values are adjusted to the mean of SAGE II and OSIRIS ozone profiles in 2002-2005 (which nearly coincide also with GOMOS data).

4.2 Target requirements

Table 22 lists selected dataset properties (Column 1), their values as set in the *a priori* data specification of Appendix D (Column 4) and the corresponding values required by users (Columns 2 and 3), as collected in the C3S Ozone Target Requirements and Gap Analysis Document (TRGAD) D11.

The gap possibly occurring between the actual values of the dataset uncertainty or stability and the corresponding specification (0) is monitored through key performance indicators (KPI) that are made available to ECMWF and project partners on the C3S Ozone dashboard to be set up.

Table 22: Specified values of selected properties of the C3S ozone vertical profile monthly mean retrieved from limb and occultation sensors (Column 4) with their user-required target and threshold values (Columns 2 and 3). M = mesosphere; US = upper stratosphere; MS = middle stratosphere; LS = lower stratosphere. When more demanding than the documented requirements, GCOS targets are mentioned in brackets.

Dataset property	**User requirement (*)**		**C3S**	
	Target (goal)	**Threshold**	**Specification (0)**	**Data products**
Geographic coverage	Global (incl. polar night)	Global	Global	all
Horizontal resolution	200 km in US/M (GCOS: 100 km)	400 km in US/M (GCOS: 200 km)	zonal average x 10° lat	all but LP_MERGED
	100 km in LS/MS	200 km in LS/MS	20° lon x 10° lat	LP_MERGED
Vertical resolution	2 km in US/M 1 km in LS/MS	4 km in US/M 2 km in LS/MS	1 km (altitude coordinate)	LMZ_MIPAS LMZ_GOMOS LMZ_SCIA LMZ_SAGE2 LMZ_SMR LMZ_OSIRIS LMZ_ACE LMZ_OMPS LMZ_SAGE-III LMZ_MERGED LP_MERGED
			1-3 km (pressure coordinate)	LMZ_HALOE LMZ_SABER LMZ_MLS

Dataset property	User requirement (*)		C3S	
	Target (goal)	Threshold	Specification (0)	Data products
Total uncertainty above 20 km (**)	4% in US/M 4% or 50 ppbv in MS	8% in US/M 8% or 100 ppbv in MS	10%	LMZ_MIPAS LMZ_GOMOS LMZ_SAGE2 LMZ_HALOE LMZ_SMR LMZ_OSIRIS LMZ_ACE LMZ_MLS LMZ_OMPS LMZ_SAGE-III LMZ_MERGED LP_MERGED
			15%	LMZ_SCIA LMZ_SABER
Total uncertainty below 20 km (**)	8% or 50 ppbv in LS	16% or 100 ppbv in LS	25%	LMZ_ACE LMZ_MLS
			30%	LMZ_MIPAS LMZ_SCIA LMZ_OSIRIS LMZ_OMPS
			35%	LMZ_MERGED LP_MERGED
			40%	LMZ_SAGE2 LMZ_HALOE
			50%	LMZ_GOMOS LMZ_SMR
Stability (**)	1% / decade	3% / decade	3% / decade	LMZ_SAGE2 LMZ_MLS
			5% / decade	LMZ_MIPAS LMZ_HALOE LMZ_OSIRIS LMZ_ACE LMZ_MERGED
			7% / decade	LMZ_GOMOS LMZ_SCIA LMZ_SABER
			8% / decade	LP_MERGED
			10% / decade	LMZ_SMR LMZ_OMPS

Dataset property	User requirement (*)		C3S	
	Target (goal)	Threshold	Specification (0)	Data products
ICDR update frequency	Daily (GCOS: 4h in LS/MS)	Weekly	Annually	LMZ_OSIRIS LMZ_ACE LMZ_SABER LMZ_MLS LMZ_OMPS LMZ_MERGED LP_MERGED

(*) As documented in the C3S Ozone Target Requirements and Gap Analysis Document (TRGAD) D11
(**) As defined in the C3S Ozone PQAD D13
(***) Requirement provided as condition on along-track sampling

4.3 Data usage information

4.3.1 Data file content, format and names

4.3.1.1 Ozone profiles retrieved from individual limb and occultation sensors (LMZ)

The monthly zonal mean (LMZ) data are recorded into monthly NetCDF files, for each instrument separately. The self-explaining filename indicates the instrument, year and month. For example, the file "200801-C3S-L3_OZONE-O3_PRODUCTS-GOMOS-ENVISAT-ALG-MONTHLY-v0001.nc" contains altitude-gridded monthly zonal mean data for GOMOS in January 2008. Analogously, "200801-C3S-L3_OZONE-O3_PRODUCTS-MLS-AURA-ALG-MONTHLY-v0003.nc" contains pressure-gridded data from MLS in January 2008. The variables that are included in the NetCDF files are reported in Table 23 for altitude-gridded files and in Table 24 for pressure-gridded files, respectively.

Table 23: The variables in altitude-gridded LMZ NetCDF files. N_{alt} and Nlat are number of altitude levels and latitude zones, respectively.

Parameter and unit	Dimensions	Description
altitude (km)	$N_{alt}\times 1$	geometric altitude
latitude_centers (degree_north)	$N_{lat}\times 1$	Centres of latitude bins: -85°: 10°:85°
ozone_ concentration (molecules/m^3)	$N_{lat}\times N_{alt}$	Monthly zonal mean ozone molecules concentration vertical profiles
standard_error_of_the_ mean (%)	$N_{lat}\times N_{alt}$	Uncertainty of the monthly zonal mean σ_{mean} (1)
sample_standard _deviation (%)	$N_{lat}\times N_{alt}$	Sample standard deviation in 1 month ×10° spatio-temporal bins, for each pressure level
mean_uncertainty_ estimate (%)	$N_{lat}\times N_{alt}$	Monthly zonal mean of error estimates (2)
inhomogeneity_in_time	$N_{lat}\times N_{alt}$	Inhomogeneity measure in time, ranges from 0 (homogeneous) to 1 (highly inhomogeneous), Sofieva et al., 2021

Parameter and unit	Dimensions	Description
inhomogneity_in_latitude	N_{lat}×N_{alt}	Inhomogeneity measure in latitude , ranges from 0 (homogeneous) to 1 (highly inhomogeneous), Sofieva et al., 2021
pressure (hPa)	N_{lat}×N_{alt}	mean air pressure corresponding to the spatiotemporal bins
temperature (K)	N_{lat}×N_{alt}	mean air temperature corresponding to the spatiotemporal bins

(1) $\sigma^2_{mean} = \frac{s^2}{N}$, where $s^2 = \langle (x_k - \bar{x})^2 \rangle$ is the sample variance. See C3S Ozone ATBD D12 , Section 3.4.3.1.

(2) $\bar{e} = \frac{1}{N}\sum e_k$, where $e_k$is the error estimate n° k. See C3S Ozone ATBD D12, Section 3.4.3.1.

Table 24: The variables in pressure-gridded LMZ NetCDF files. N_{alt} and N_{lat} are pressures levels and latitude zones, respectively.

Parameter and unit	Dimensions	Description
air_pressure (hPa)	N_{alt}×1	The vertical coordinate
latitude_centers (degree_north)	N_{lat} ×1	Centres of latitude bins: -85°: 10°:85°
ozone_mixing_ratio	N_{lat}×N_{alt}	Monthly zonal mean ozone mixing ratio vertical profiles
standard_error_of_the_ mean (%)	N_{lat}×N_{alt}	Uncertainty of the monthly zonal mean σ_{mean} (1)
sample_standard _deviation (%)	N_{lat}×N_{alt}	Sample standard deviation in 1 month ×10° spatio-temporal bins, for each pressure level
mean_uncertainty_ estimate (%)	N_{lat}×N_{alt}	Monthly zonal mean of error estimates (2)
inhomogeneity_in_time	N_{lat}×N_{alt}	Inhomogeneity measure in time
inhomogneity_in_latitude	N_{lat}×N_{alt}	Inhomogeneity measure in latitude
temperature (K)	N_{lat}×N_{alt}	mean air temperature corresponding to the spatiotemporal bins
altitude (km)	N_{lat}×N_{alt}	mean altitude corresponding to the spatiotemporal bins

(1) $\sigma^2_{mean} = \frac{s^2}{N}$, where $s^2 = \langle (x_k - \bar{x})^2 \rangle$ is the sample variance. See C3S Ozone ATBD D12, Section 3.4.3.1.

(2) $\bar{e} = \frac{1}{N}\sum e_k$, where $e_k$is the error estimate n° k. See C3S Ozone ATBD D12 Section 3.4.3.1.

4.3.1.2 Merged monthly zonal mean ozone profiles retrieved from limb and occultation sensors (LMZ_MERGED)

The merged monthly zonal mean data are recorded into monthly NetCDF-4 files. Deseasonalised anomalies and ozone concentration profiles are provided in separate files. The altitude range for LMZ-merged is 10 -50 km and the latitude zones are 10° wide from 90°S to 90°N. The variables included in the NetCDF files are reported in Table 25 for ozone anomalies and in Table 26 for ozone concentrations.

Table 25: The variables in LMZ_merged NetCDF files with deseasonalized anomalies. N_{alt} and Nlat are number of altitude levels and latitude zones, respectively. N_{instru} is the number of instruments.

	Parameter and unit	Dimensions	Description
General parameters	altitude (km)	N_{alt}×1	geometric altitude
	latitude_centers (degrees_north)	N_{lat} ×1	Centers of latitude bins: -85°: 10°:85°
	instruments	N_{instru}×1	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_{alt}×N_{lat}	Merged deseasonalized anomalies, see ATBD for details
	uncertainty_of_ merged_ozone_anomaly (%)	N_{alt}×N_{lat}	Uncertainty of the merged data
	pressure (hPa)	N_{alt}×N_{lat}	Mean pressure corresponding to spatiotemporal bins
	Temperature (K)	N_{alt}×N_{lat}	Mean temperature corresponding to spatiotemporal bins
Individual datasets	ozone_anomaly_instrument (%)	N_{alt}×N_{lat}×N_{instru}	Deseasonalized anomalies of ozone from individual instruments
	Uncertainty_of_ozone_anomaly_instrument (%)	N_{alt}×N_{lat}×N_{instru}	Uncertainty of deseasonalized anomalies individual datasets

Table 26: The variables in LMZ_merged NetCDF files with ozone concentrations. N_{alt} and Nlat are number of altitude levels and latitude zones, respectively. N_{instru} is the number of instruments.

	Parameter and unit	Dimensions	Description
General parameters	altitude (km)	N_{alt}×1	geometric altitude
	latitude_centers (degrees_north)	N_{lat} ×1	Centers of latitude bins: -85°: 10°:85°
	instruments	N_{instru}×1	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	merged_ozone_concentration (molecules/m^3)	N_{alt}×N_{lat}	Vertical profiles of merged monthly zonal mean ozone molecular concentration.
	uncertainty_of_ merged_ozone_concentration(molecules/m^3)	N_{alt}×N_{lat}	Uncertainty of the merged data

	Parameter and unit	Dimensions	Description
	pressure (hPa)	$N_{alt} \times N_{lat}$	Mean pressure corresponding to spatiotemporal bins
	Temperature (K)	$N_{alt} \times N_{lat}$	Mean temperature corresponding to spatiotemporal bins

4.3.1.3 Merged monthly mean ozone profiles with resolved longitudinal structure (LP_MERGED)

The merged monthly zonal mean data with resolved longitudinal structure are recorded in monthly NetCDF-4 files. Deseasonalised anomalies and ozone concentration profiles are provided in separate files. The altitude range for LP-MERGED dataset is 10 -50 km, the data are averaged over 10° x 20° latitude-longitude zones. The variables included in the NetCDF files with deseasonalised anomalies and ozone concentrations are reported in Table 27 and Table 28 respectively.

Table 27: The variables in LP_MERGED NetCDF file with deseasonalized anomalies. N_{alt}, N_{lat} , N_{lon} are number of altitude levels, latitude and longitude zones, respectively. N_{instru} is the number of instruments.

	Parameter and unit	Dimensions	Description
General parameters	altitude (km)	$N_{alt} \times 1$	geometric altitude
	latitude_centers (degrees_north)	$N_{lat} \times 1$	Centres of latitude bins: -85°: 10°:85°
	longitude_centers (degree_east)	$N_{lon} \times 1$	Centres of longitude bins: -170°:20°:170°
	instruments	$N_{instru} \times 1$	A dimension for individual datasets, instrument order 1-GOMOS, 2-MIPAS, 3-SCIAMACHY, 4-OSIRIS, 5-MLS, 6- OMPS-LP
Merged data	merged_ozone_anomaly (%)	$N_{alt} \times N_{lat} \times N_{lon}$	Merged deseasonalized anomalies, see ATBD for details
	uncertainty_of_ merged_ozone_anomaly (%)	$N_{alt} \times N_{lat} \times N_{lon}$	Uncertainty of the merged data
	pressure (hPa)	$N_{alt} \times N_{lat} \times N_{lon}$	Mean pressure corresponding to spatiotemporal bins
	Temperature (K)	$N_{alt} \times N_{lat} \times N_{lon}$	Mean temperature corresponding to spatiotemporal bins
Individual datasets	ozone_anomaly_instrument (%)	$N_{alt} \times N_{lat} \times N_{lon} \times N_{instru}$	Deseasonalized anomalies of ozone from individual instruments
	Uncertainty_of_ozone anomaly_instrument (%)	$N_{alt} \times N_{lat} \times N_{lon} \times N_{instru}$	Uncertainty of deseasonalized anomalies individual datasets

Table 28. The variables in LP_MERGED NetCDF file with ozone concentrations. N_{alt}, N_{lat} , N_{lon} are number of altitude levels, latitude and longitude zones, respectively. N_{instru} is the number of instruments.

	Parameter and unit	Dimensions	Description
General parameters	altitude (km)	N_{alt}×1	geometric altitude
	latitude_centers (degrees_north)	N_{lat} ×1	Centres of latitude bins: -85°: 10°:85°
	longitude_centers (degree_east)	N_{lon} ×1	Centres of longitude bins: -170°:20°:170°
	instruments	N_{instru}×1	A dimension for individual datasets, instrument order 1-GOMOS, 2-MIPAS, 3-SCIAMACHY, 4-OSIRIS, 5-MLS, 6- OMPS-LP
Merged data	merged_ozone_concentration (molecules/m^3)	N_{alt}×N_{lat}×N_{lon}	Vertical profiles of merged monthly zonal mean ozone molecular concentration.
	uncertainty_of_ merged_ozoneconcentrations (molecules/m^3)	N_{alt}×N_{lat}×N_{lon}	Uncertainty of the merged data
	pressure (hPa)	N_{alt}×N_{lat}×N_{lon}	Mean pressure corresponding to spatiotemporal bins
	Temperature (K)	N_{alt}×N_{lat}×N_{lon}	Mean temperature corresponding to spatiotemporal bins
Individual datasets	ozone_concentration_instrument (molecules m^{-3})	N_{alt}×N_{lat}×N_{lon} ×N_{instru}	Gridded ozone profiles for individual instruments
	Uncertainty_of_ozone_concentration_instrument (%)	N_{alt}×N_{lat}×N_{lon} ×N_{instru}	Random uncertainties of the gridded ozone profiles for individual instruments

4.3.2 Data disclaimer

Stratospheric ozone profiles are delivered. The quality of limb ozone profiles is significantly lower below the tropopause.

5. Data access information

The Level-3 and Level-4 data products generated by the C3S Ozone project partners are stored as they are produced in the Ozone CDR Central Data Base hosted at BIRA-IASB, where they are validated. At each delivery date, products are transferred from BIRA-IASB to DLR, then fed into the C3S climate data store (CDS) at ECMWF, from where they are made available to users via the CDS interface [2].

Essential documents accompany the data. They are provided to ECMWF to be made available to the users via the C3S CDS interface. They can be found on the CDS website under the “Documentation”

[2] https://cds.climate.copernicus.eu/cdsapp#!/dataset/satellite-ozone-v1?tab=form (last accessed 23/04/2024)

tab, from where they can be downloaded. Visualization of the netCDF files can be conducted with standard tools (e.g. Panoply distributed by NASA)

The primary source of information on C3S ozone products is this Product User Guide and Specification (PUGS).

The C3S Ozone Algorithm Theoretical Basis Document (ATBD) D12 provides an in-depth description of the algorithms applied to derive the delivered products, including the observation techniques and the data input and output.

The C3S Ozone Product Quality Assurance Document (PQAD) D13 describes the validation method applied to the data while the Product Quality Assessment Report (PQAR) D14 gives an account of the validation results and provides an assessment of the data compliance with user requirements presented in the Target Requirements and Gap Analysis Document (TRGAD) D11.

User queries about C3S ozone data are addressed to the C3S Service Desk (https://climate.copernicus.eu/c3s-user-service-desk). The front-end user support on C3S data is provided by the CDS team based on a list of expected frequently asked questions (FAQ) and their answers. When the answer to a question requires technical explanations that cannot be immediately provided by the Copernicus User Support (CUS) team, the question is forwarded to the C3S specialised support agent who ensures that each ozone product-related query is redirected to the most appropriate science team member, i.e. data developers or suppliers providing the second line of expertise. Provider details of the data suppliers can be found in Table 29. Details of the upstream Level-2 data developers are provided in Table 30.

Table 29: C3S ozone L-3 and L-4 data provider details.

L-3 ozone total columns retrieved from UV nadir sensors					
Data product provider	German Aerospace Centre (DLR)				
Data product names	TC_GOME TC_SCIA	TC_GOME2A TC_GOME2B	TC_OMI TC_OMPS	TC_GOME2C TC_S5P	TC_GTO-ECV
L-4 ozone total column retrieved from UV nadir sensors (data assimilation)					
Data product provider	Royal Netherlands Meteorological Institute (KNMI)				
Data product name	TC_MSR				
L-3 ozone total and tropospheric columns retrieved from IASI					

Data product provider	Université Pierre et Marie Curie / Laboratoire Atmosphères et Observations Spatiales (UPMC/LATMOS)				
Data product name	TC_IASI-A TC_IASI-B TC_IASI-C	06TC_IASI-A 06TC_IASI-B 06TC_IASI-C			
L-3 ozone profiles retrieved from UV nadir sensors					
Data product provider	Royal Netherlands Meteorological Institute (KNMI)				
Data product names	NP_GOME NP_SCIA	NP_GOME2A NP_GOME2B	NP_OMI		
L-3 merged ozone profiles retrieved from UV nadir sensors					
Data product provider	German Aerospace Centre (DLR)				
Data product names	NP_GOP-ECV				
L-3 ozone profiles retrieved from limb and occultation sensors					
Data product provider	Finnish Meteorological Institute (FMI)				
Data product name(s)	LMZ_MIPAS LMZ_GOMOS LMZ_SCIA	LMZ_SAGE2 LMZ_HALOE LMZ_SMR	LMZ_OSIRIS LMZ_ACE LMZ_SABER	LMZ_MLS LMZ_OMPS-SASK LMZ_OMPS-UB	LMZ_SAGE3 LP_MERGED LMZ_MERGED

Table 30: Level-2 data developer details.

L-2 ozone total columns retrieved from UV nadir sensors					
Data product developer	Royal Belgian Institute for Space Aeronomy (IASB-BIRA)				
Derived L-3 data product names	TC_GOME TC_SCIA	TC_GOME2A TC_GOME2B	TC_OMI TC_OMPS	TC_GOME2C TC_S5P	TC_GTO-ECV
L-2 ozone total and tropospheric columns retrieved from IASI					

Data product developer	Université Pierre et Marie Curie / Laboratoire Atmosphères, Milieux, Observations Spatiales (UPMC/LATMOS)			
Derived L-3 data product name	TC_IASI-A TC_IASI-B TC_IASI-C	06TC_IASI-A 06TC_IASI-B 06TC_IASI-C		
L-2 ozone profiles retrieved from UV nadir sensors				
Data product developer	Science and Technology Facilities Council / Rutherford Appleton Laboratory (STFC/RAL)			
Derived L-3 data product names	NP_GOME NP_SCIA	NP_GOME2A NP_GOME2B	NP_OMI	
L-2 ozone profiles retrieved from limb and occultation sensors				
Data product developer	Universität Bremen / Institut für Umweltphysik (UiB/IUP)			
Derived L-3 data product names	LMZ_MIPAS LMZ_GOMOS LMZ_SCIA LMZ_SAGE2	LMZ_HALOE LMZ_SMR LMZ_OSIRIS LMZ_SAGE3	LMZ_ACE LMZ_SABER LMZ_MLS LMZ_OMPS-SASK	LMZ_OMPS-UB LMZ_MERGED LP_MERGED

Appendix A. Specifications for the L-3 and L-4 ozone total columns retrieved from UV-nadir sensors

This group of C3S ozone products includes Level-3 and Level-4 monthly mean total columns retrieved from UV nadir satellite observations. Data are from individual sensors, merged or the outcome of multi-sensor reanalysis by data assimilation (see dataset description in Section 0). The data product specification is provided in Table 31.

For the different versions archived in the CDS, the time periods covered by each of them and the occasionally missing months, please refer to Table 3, Page 23

Table 31: Specification of the Level 3 and Level 4 ozone total column monthly mean from UV-nadir sensors.

Property	**Specification**	
Data product names	TC_GOME TC_SCIA TC_GOME2A TC_GOME2B TC_GOME2C TC_OMI TC_OMPS TC_S5P TC_GTO-ECV TC_MSR	
Data class	Earth Observation Data	
Originating satellite/instrument systems	TC_GOME	ERS-2/GOME
	TC_SCIA	Envisat/SCIAMACHY
	TC_GOME2A	Metop-A/GOME-2
	TC_GOME2B	Metop-B/GOME-2
	TC_GOME2C	Metop-C/GOME-2
	TC_OMI	Aura/OMI
	TC_OMPS	Suomi NPP/OMPS-NM
	TC_S5P	Sentinel-5p/TROPOMI
	TC_GTO-ECV	All the above, except SNPP/OMPS-NM
	TC_MSR	All the above + Nimbus4/BUV, Nimbus7/TOMS, EP/TOMS, SBUV series
ATBD	C3S Ozone Algorithm Theoretical Document D12	
Main variable physical nature & unit	Monthly mean ozone total column (molecules m^{-2})	
Processing level	TC_GOME	3
	TC_SCIA	3
	TC_GOME2A	3
	TC_GOME2B	3
	TC_GOME2C	3
	TC_OMI	3
	TC_OMPS	3
	TC_S5P	3

	TC_GTO-ECV	3
	TC_MSR	4
Temporal coverage (all versions)	TC_GOME	06.1995 - 07.2011
	TC_SCIA	08.2002 - 04.2012
	TC_GOME2A	01.2007 – 10.2021
	TC_GOME2B	01.2013 – today
	TC_GOME2C	07.2019 – today
	TC_OMI	10.2004 – today
	TC_OMPS	01.2012 – today
	TC_S5P	05.2018 – today
	TC_GTO-ECV	07.1995 – today
	TC_MSR	04.1970 – today
Temporal resolution	Monthly	
Geographic coverage	Global	
Horizontal resolution	1° longitude x 1° latitude	
Maximum total uncertainty	TC_GOME	5%
	TC_SCIA	3%
	TC_GOME2A	3%
	TC_GOME2B	3%
	TC_GOME2C	3%
	TC_OMI	3%
	TC_OMPS	3%
	TC_S5P	3%
	TC_GTO-ECV	3%
	TC_MSR	2%
Stability (maximum drift)	1% / decade	
Update frequency	TC_GOME2B	Quarterly
	TC_GOME2C	Quarterly
	TC_OMI	Quarterly
	TC_OMPS	Quarterly
	TC_S5P	Quarterly
	TC_GTO-ECV	Semi-annually
	TC_MSR	Annually
Update delay	TC_GOME2B	4 months
	TC_GOME2C	4 months
	TC_OMI	4 months
	TC_OMPS	4 months
	TC_S5P	4 months
	TC_GTO-ECV	4 months
	TC_MSR	3 months
Data format	CF-compliant NetCDF	

Appendix B. Specifications for the L-3 ozone total and tropospheric columns retrieved from IASI

This family of C3S ozone products includes Level-3 monthly mean total and tropospheric (0 to 6 km) columns retrieved from observations by IASI (see dataset description in Section 0). The data product specification is provided in Table 32.

The time periods covered by the different versions archived in the CDS are reported in Table 9. There is no IASI-A O_3 data available between April and September 2015 (TC_IASI-A & 06TC_IASI-A, CDS version 0001) because of a temporary issue related to alignment in the IASI-A L1 data.

Table 32: Specification of the Level 3 ozone total and tropospheric column monthly mean from IASI.

Property	**Specification**	
Data product names	TC_IASI-A TC_IASI-B TC_IASI-C 06TC_IASI-A 06TC_IASI-B 06TC-IASI-C	
Data class	Earth Observation Data	
Originating satellite/instrument system	TC_IASI-A	Metop-A/IASI
	06TC_IASI-A	
	TC_IASI-B	Metop-B/IASI
	06TC_IASI-B	
	TC_IASI-C 06TC_IASI-C	Metop-C/IASI
ATBD	C3S Ozone Algorithm Theoretical Document D12	
Main variable physical nature & unit	TC_IASI-A	Monthly mean ozone total column (molecules/m^2)
	TC_IASI-B	
	TC_IASI-C	
	06TC_IASI-A	Monthly mean ozone tropospheric column (molecules/m^2) (between the ground and the altitude of 6 km)
	06TC_IASI-B	
	06TC_IASI-C	
Processing level	3	
Temporal coverage	TC_IASI-A	10.2007 – 08.2021
	06TC_IASI-A	
	TC_IASI-B	05.2013 - today
	06TC_IASI-B	
	TC_IASI-C	10.2019 – today
	06TC_IASI-C	
Temporal resolution	Monthly	
Geographic coverage	Global	
Horizontal resolution	1° longitude x 1° latitude	
Maximum total uncertainty	TC_IASI-A	3%
	TC_IASI-B	
	TC_IASI-C	

	06TC_IASI-A	30%
	06TC_IASI-B	
	06TC_IASI-C	
Stability (maximum drift)	TC_IASI-A	1% / decade
	TC_IASI-B	3% / decade
	TC_IASI-C	3% / decade
	06TC_IASI-A	20% / decade
	06TC_IASI-B	20% / decade
	06TC_IASI-C	20% / decade
Update frequency	Quarterly	
Update delay	1 month	
Data format	CF-compliant NetCDF	

Appendix C. Specifications for the L-3 ozone profiles retrieved from UV-nadir sensors

This family of C3S ozone products includes Level-3 monthly mean profiles retrieved from UV nadir satellite observations. Data are from five individual sensors (see dataset description in Section 0). In addition a merged product is provided. The data product specification is provided in Table 33. The drift and total uncertainty ceilings are based on the error budget of the Level 2 datasets D8.

Table 33: Specification of the Level 3 ozone profile monthly mean from UV-nadir sensors.

Property	**Specification**	
Data product names	NP_GOME NP_SCIA NP_GOME2A NP_GOME2B NP_OMI NP_GOP-ECV	
Data class	Earth Observation Data	
Originating satellite/instrument systems	NP_GOME	ERS-2/GOME
	NP_SCIA	Envisat/SCIAMACHY
	NP_GOME2A	Metop-A/GOME-2
	NP_GOME2B	Metop-B/GOME-2
	NP_OMI	Aura/OMI
	NP_GOP-ECV	ERS-2/GOME Envisat/SCIAMACHY Metop-A/GOME-2 Metop-B/GOME-2 Aura/OMI
ATBD	C3S Ozone Algorithm Theoretical Document D12	
Main variable physical nature & unit	Monthly mean ozone molecular number density (cm^{-3}) Monthly mean ozone volume mixing ratio (ppmv) Monthly mean ozone partial column (molecules m^{-2})	
Processing level	3	
Temporal coverage (all versions)	NP_GOME	06.1995 - 06.2011
	NP_SCIA	08.2002 - 04.2012
	NP_GOME2A	01.2007 - 10.2021
	NP_GOME2B	04.2013 – 06.2023
	NP_OMI	10.2004 – 10.2021
	NP_GOP-ECV	07.1995 – 10.2021
Temporal resolution	Monthly	
Geographic coverage	Global	
Horizontal resolution	1° longitude x 1° latitude (5° longitude x 5° latitude for NP_GOP-ECV)	
Vertical coordinate and unit	pressure (hPa)	
Vertical coverage	from surface to TOA	

Vertical grid	levels at surface and at 450, 170, 100, 50, 30, 20, 10, 5, 3, 2, 1, 0.5, 0.3, 0.17, 0.1, 0.05, 0.03, 0.017 and 0.01 hPa. (i.e. the L2 retrieval levels)	
Maximum total uncertainty	Above tropopause	20%
	Below tropopause	30%
Stability (maximum drift)	NP_GOME	3% / decade
	NP_SCIA	20% / decade
	NP_GOME2A	20% / decade
	NP_GOME2B	20% / decade
	NP_OMI	3% / decade
ICDR update frequency	NP_GOME2B	Annually
	NP_OMI	Annually
ICDR update delay	NP_GOME2B	4 months
	NP_OMI	4 months
Data format	CF-compliant NetCDF	

Appendix D. Specifications for the L-3 ozone profiles retrieved from limb and occultation sensors

This family of C3S ozone products includes Level-3 monthly mean profiles retrieved from limb and occultation satellite observations. Data are from 13 individual sensors with two additional merged products (see dataset description in Section 0). The data products specification is provided in Table 34. The drift and total uncertainty ceilings are based on the error budget of the Level 2 datasets D8.

For the different versions archived in the CDS, the time periods covered by each of them and the occasionally missing months, please refer to Table 19, Page 41.

Table 34: Specification of the Level 3 ozone profile monthly mean from limb and occultation sensors.

Property	**Specification**	
Data product names	LMZ_MIPAS LMZ_GOMOS LMZ_SCIA LMZ_SAGE2 LMZ_HALOE LMZ_SMR LMZ_OSIRIS LMZ_ACE LMZ_SABER LMZ_MLS LMZ_OMPS-SASK LMZ_OMPS-UB LMZ_SAGE-III LMZ_MERGED LP_MERGED	
Data class	Earth Observation Data	
Originating satellite/instrument systems	LMZ_MIPAS	Envisat/MIPAS
	LMZ_GOMOS	Envisat/GOMOS
	LMZ_SCIA	Envisat/SCIAMACHY
	LMZ_SAGE2	ERBS/SAGE-2
	LMZ_HALOE	UARS/HALOE
	LMZ_SMR	Odin/SMR
	LMZ_OSIRIS	Odin/OSIRIS
	LMZ_ACE	SciSat/ACE-FTS
	LMZ_SABER	TIMED/SABER
	LMZ_MLS	Aura/MLS
	LMZ_SAGE-III	ISS/SAGE-III
	LMZ_OMPS-SASK	Suomi NPP/OMPS-LP
	LMZ_OMPS-UB	Suomi NPP/OMPS-LP

	LMZ_MERGED	Envisat/MIPAS Envisat/GOMOS Envisat/SCIAMACHY ERBS/SAGE-2 Odin/OSIRIS SciSat/ACE-FTS Suomi NPP/OMPS-LP ISS/SAGE-III Spot4/POAM-III
	LP_MERGED	Envisat/MIPAS Envisat/GOMOS Envisat/SCIAMACHY Odin/OSIRIS Suomi NPP/OMPS-LP Aura/MLS
ATBD	C3S Ozone Algorithm Theoretical Document D12	
Main variable physical nature & unit	Monthly mean ozone volume mixing ratio (ppmv) Monthly mean ozone molecular concentration (molecules.cm^{-3}) For the merged products: ozone concentration anomaly (molecules.cm^{-3})	
Processing level	3	
Temporal coverage	LMZ_MIPAS	07.2002 - 04.2012
	LMZ_GOMOS	08.2002 -12.2011
	LMZ_SCIA	08.2002 - 03.2012
	LMZ_SAGE2	10.1984 - 08.2005
	LMZ_HALOE	10.1991 - 09.2005
	LMZ_SMR	07.2001 - 08.2014
	LMZ_OSIRIS	11.2001 - today
	LMZ_ACE	02.2004 - today
	LMZ_SABER	01.2002 - today
	LMZ_MLS	08.2004 - today
	LMZ_OMPS-SASK	02.2012 – today
	LMZ_OMPS-UB	02.2012 – today
	LMZ_SAGE-III	06.2017 - today
	LMZ_MERGED	10.1984 - today
	LP_MERGED	11.2001 - today
Temporal resolution	Monthly	
Geographic coverage	Global	
Longitude resolution	LMZ_MIPAS	360° (zonal average)
	LMZ_GOMOS	360° (zonal average)
	LMZ_SCIA	360° (zonal average)
	LMZ_SAGE2	360° (zonal average)
	LMZ_HALOE	360° (zonal average)
	LMZ_SMR	360° (zonal average)
	LMZ_OSIRIS	360° (zonal average)
	LMZ_ACE	360° (zonal average)
	LMZ_SABER	360° (zonal average)
	LMZ_MLS	360° (zonal average)

	LMZ_SAGE-III	360° (zonal average)
	LMZ_OMPS-UB	360° (zonal average)
	LMZ_OMPS-SASK	360° (zonal average)
	LMZ_MERGED	360° (zonal average)
	LP_MERGED	20°
Latitude resolution	10°	
Vertical coordinate and unit	LMZ_MIPAS	altitude (km)
	LMZ_GOMOS	altitude (km)
	LMZ_SCIA	altitude (km)
	LMZ_SAGE2	altitude (km)
	LMZ_SAGE3	altitude (km)
	LMZ_HALOE	pressure (hPa)
	LMZ_SMR	altitude (km)
	LMZ_OSIRIS	altitude (km)
	LMZ_ACE	altitude (km)
	LMZ_SABER	pressure (hPa)
	LMZ_MLS	pressure (hPa)
	LMZ_OMPS-UB	altitude (km)
	LMZ_OMPS-SASK	altitude (km)
	LMZ_MERGED	altitude (km)
	LP_MERGED	altitude (km)
Vertical coverage	LMZ_MIPAS	6-68 km
	LMZ_GOMOS	10-105 km
	LMZ_SCIA	5-65 km
	LMZ_SAGE2	5-65 km
	LMZ_HALOE	500 – 0.02hPa
	LMZ_SMR	15-65 km
	LMZ_OSIRIS	10-59 km
	LMZ_ACE	6-94 km
	LMZ_SABER	50 – 0.1hPa
	LMZ_MLS	500 – 0.02hPa
	LMZ_OMPS-SASK	7-58 km
	LMZ_OMPS-UB	7-58 km
	LMZ_SAGE-III	5-65 km
	LMZ_MERGED	10-50 km
	LP_MERGED	10-50 km
Vertical resolution or levels	LMZ_MIPAS	1 km
	LMZ_GOMOS	1 km
	LMZ_SCIA	1 km
	LMZ_SAGE2	1 km
	LMZ_HALOE	1-3 km
	LMZ_SMR	1 km
	LMZ_OSIRIS	1 km
	LMZ_ACE	1 km
	LMZ_SABER	1-3 km
	LMZ_MLS	1-3 km
	LMZ_SAGE-III	1 km

	LMZ_OMPS-UB	1 km	
	LMZ_OMPS-SASK	1 km	
	LMZ_MERGED	1 km	
	LP_MERGED	1 km	
Maximum total uncertainty		Above 20 km	Below 20 km
	LMZ_MIPAS	10%	30%
	LMZ_GOMOS	10%	50%
	LMZ_SCIA	15%	30%
	LMZ_SAGE2	10%	40%
	LMZ_HALOE	10%	40%
	LMZ_SMR	10%	50%
	LMZ_OSIRIS	10%	30%
	LMZ_ACE	10%	25%
	LMZ_SABER	15%	/
	LMZ_MLS	10%	25%
	LMZ_SAGE-III	10%	30%
	LMZ_OMPS-SASK	10%	30%
	LMZ_OMPS-UB	10%	30%
	LMZ_MERGED	10%	35%
	LP_MERGED	10%	35%
Stability (maximum drift)	LMZ_MIPAS	5% / decade	
	LMZ_GOMOS	7% / decade	
	LMZ_SCIA	7% / decade	
	LMZ_SAGE2	3% / decade	
	LMZ_HALOE	5% / decade	
	LMZ_SMR	10% / decade	
	LMZ_OSIRIS	5% / decade	
	LMZ_ACE	5% / decade	
	LMZ_SABER	7% / decade	
	LMZ_MLS	3% / decade	
	LMZ_SAGE-III	5% / decade	
	LMZ_OMPS-SASK	10% / decade	
	LMZ_OMPS-UB	10% / decade	
	LMZ_MERGED	5% / decade	
	LP_MERGED	8% / decade	
ICDR update frequency	LMZ_OSIRIS	Annually	
	LMZ_ACE	Annually	
	LMZ_SABER	Annually	
	LMZ_MLS	Annually	
	LMZ_SAGE-III	Annualy	
	LMZ_OMPS-SASK	Annually	
	LMZ_OMPS-UB	Annually	
	LMZ_MERGED	Annually	
	LP_MERGED	Annually	
ICDR update delay	LMZ_OSIRIS	3 months	
	LMZ_ACE	3 months	
	LMZ_SABER	3 months	

	LMZ_MLS	3 months
	LMZ_SAGE-III	3 months
	LMZ_OMPS-SASK	3 months
	LMZ_OMPS-UB	3 months
	LMZ_MERGED	3 months
	LP_MERGED	3 months
Data format	CF-compliant NetCDF	

Appendix E. Data product overview and version history.

The temporal coverage indicated for each product in Table 35 is the overall time period over which data are available for that product. In practice, different versions of the product may span only parts of this time period. This is especially true for ICDRs. In the CDS, only the most recently updated version of the latter is mentioned as being an ICDR, previous versions being considered as completed CDRs. An overview of the different versions together with their temporal coverage is shown in Table 36.

Table 35: List of the C3S ozone data products available from the C3S CDS (February 2024). All products cover the globe and have a monthly temporal resolution. Data are provided in the NetCDF format. For the merged products the sensors that are included are listed below the table. Therefore in the Sensor column the merged products are indicated with a number that refers to the corresponding note below the table.

Product name	Product definition	Sensor(s)	Processing level	Product type	Overall temporal coverage	Update frequency	Spatial resolution	Uncertainty information	Provision & provenance
TC_GOME	Total ozone column	GOME	3	CDR	06.1995 - 07.2011	N/A	1°x1°	Random and smoothing error	BIRA/DLR
TC_SCIA		SCIAMACHY	3	CDR	08.2002 - 04.2012	N/A	1°x1°		BIRA/DLR
TC_GOME2A		GOME-2A	3	CDR	01.2007 - 10.2021	N/A	1°x1°		BIRA/DLR
TC_GOME2B		GOME-2B	3	ICDR	01.2013 -	Quarterly with 4 months delay	1°x1°		BIRA/DLR
TC_GOME2C		GOME-2C	3	ICDR	07.2019 -		1°x1°		BIRA/DLR
TC_OMI		OMI	3	ICDR	10.2004 -		1°x1°		BIRA/DLR

TC_OMPS		OMPS-NM	3	ICDR	01.2012 -		1°x1°		BIRA/DLR
TC_S5P		S5P-TROPOMI	3	ICDR	05.2018 -		1°x1°		DLR
TC_GTO-ECV		(4)	3	ICDR	07.1995 -	Semi-annually with 4 months delay	1°x1°	Random and sampling error	BIRA/DLR
TC_MSR		(1)	4	ICDR	04.1970 -	Annually with 3 months delay	1°x1°	Forecast error covariance	KNMI
TC_IASI-A	Total and tropospheric ozone	IASI-A	3	CDR	10.2007 - 08.2021	N/A	1°x1°	Random error	LATMOS
06TC_IASI-A		IASI-A	3	CDR	10.2007 - 08.2021	N/A	1°x1°	Random error	LATMOS
TC_IASI-B		IASI-B	3	ICDR	05.2013 -	Quarterly with 1 month delay	1°x1°	Random error	LATMOS
TC_IASI-C		IASI-C	3	ICDR	10.2019 -		1°x1°	Random error	LATMOS
06TC_IASI-B		IASI-B	3	ICDR	05.2013 -		1°x1°	Random error	LATMOS
06TC_IASI-C		IASI-C	3	ICDR	10.2019 -		1°x1°	Random error	LATMOS
NP_GOME	Ozone profile (nadir)	GOME	3	CDR	06.1995 - 06.2011	N/A	1°x1°	Random and smoothing error	RAL/KNMI
NP_SCIA		SCIAMACHY	3	CDR	08.2002 - 04.2012	N/A	1°x1°		RAL/KNMI
NP_GOME2A		GOME-2A	3	CDR	01.2007 - 10.2021	N/A	1°x1°		RAL/KNMI
NP_GOME2B		GOME-2B	3	ICDR	04.2013 –	Annually with 4 months delay	1°x1°		RAL/KNMI
NP_OMI		OMI	3	ICDR	10.2004 -		1°x1°		RAL/KNMI
NP_GOP-ECV		(5)	3	ICDR	07.1995 – 10.2021	N/A	5°x5°		KNMI/DLR
LMZ_MIPAS	Ozone profile (limb)	MIPAS	3	CDR	07.2002 - 04.2012	N/A	10° lat zones	Random and sampling error	UNI-HB/FMI
LMZ_GOMOS		GOMOS	3	CDR	08.2002 - 12.2011	N/A	10° lat zones		UNI-HB/FMI

LMZ_SCIA		SCIAMACHY	3	CDR	08.2002 - 03.2012	N/A	10° lat zones		UNI-HB/FMI
LMZ_SAGE2		SAGE-2	3	CDR	10.1984 - 08.2005	N/A	10° lat zones		UNI-HB/FMI
LMZ_HALOE		HALOE	3	CDR	10.1991 - 09.2005	N/A	10° lat zones		UNI-HB/FMI
LMZ_SMR (*)		SMR (*)	3	CDR (*)	07.2001 - 08.2014 (*)	N/A (*)	10° lat zones		UNI-HB/FMI
LMZ_OSIRIS		OSIRIS	3	ICDR	11.2001 -	Annually with 3 months delay	10° lat zones		UNI-HB/FMI
LMZ_ACE		ACE	3	ICDR	02.2004 -		10° lat zones		UNI-HB/FMI
LMZ_SABER		SABER	3	ICDR	01.2002 -		10° lat zones		UNI-HB/FMI
LMZ_MLS		MLS	3	ICDR	08.2004 -		10° lat zones		UNI-HB/FMI
LMZ_OMPS-SASK		OMPS-LP	3	ICDR	02.2012 -		10° lat zones		UNI-HB/FMI
LMZ_OMPS-UB		OMPS-LP	3	ICDR	02.2012 -		10° lat zones		UNI-HB/FMI
LMZ_SAGE-III		SAGE-III	3	ICDR	06.2017 -		10° lat zones		UNI-HB/FMI
LMZ_MERGED		(2)	3	ICDR	10.1984 -		10° lat zones		FMI
LP_MERGED		(3)	3	ICDR	11.2001 -		10°x20°		FMI

TC Total column monthly gridded average product
NP Nadir profile monthly gridded average product
LP Limb profile monthly gridded average product
LMZ Limb monthly zonal profile average product
(*) SMR is still in operation but the L1 data processing has been interrupted in 2014. It may resume later with the reprocessing of the Odin entire data record.
(1) Merged/assimilated product based on GOME, SCIAMACHY, OMI, GOME-2A/B/C, BUV-Nimbus4, TOMS-Nimbus7, TOMS-EP, SBUV-7, -9, -11, -14, -16, -17, -18, -19, OMPS and TROPOMI
(2) Monthly zonal mean merged product (concentration and concentration anomaly) based on MIPAS, GOMOS, SCIAMACHY, SAGE-2, OSIRIS, ACE and OMPS
(3) Latitude-longitude gridded merged product (concentration and concentration anomaly) based on MIPAS, GOMOS, SCIAMACHY and OSIRIS.
(4) Merged product based on GOME, SCIAMACHY, GOME-2A/B/C, OMI and S5P
(5) Merged product based on GOME, SCIAMACHY, GOME-2A/B, and OMI

Table 36: Version history together with the temporal coverage for the C3S ozone data products

Product name	Version	Temporal coverage	comments
TC_GOME	v0100	06.1995 - 07.2011	
TC_SCIA	v0100	08.2002 - 04.2012	
TC_GOME2A	v0100	01.2007 - 10.2021	
TC_GOME2B	V0100	01/2013-10/2018	
	V0101	07/2018-	Update of L2
TC_GOME2C	V0100	07/2019-	
TC_OMI	V0100	10/2004-01/2019	
	V0101	01/2017-	stricter row filtering
TC_OMPS	V0100	01/2012-	
TC_S5P	V0100	05/2018-	
TC_GTO-ECV	V0100	07/1995-06/2017	
	V0200	01/2007-06/2018	Update of correction factors (applies to GOME-2A/-2B) and extension in time
	V0300	01/2007-10/2018	Update of correction factors (applies to GOME-2A/-2B) and extension in time
	V0400	01/2007-07/2019	Update of correction factors (applies to GOME-2A/-2B) and extension in time
	V0500	01/2007-10/2019	Update of correction factors (applies to GOME-2A/-2B) and extension in time
	V0600	01/2007-04/2020	Update of correction factors (applies to GOME-2A/-2B) and extension in time
	V0700	01/2007-10/2020	Update of correction factors (applies to GOME-2A/-2B) and extension in time
	V0800	01/2007-10/2021	Update of correction factors (applies to GOME-2A/-2B), inclusion of GOME-2C and TROPOMI in GTO-ECV and extension in time
	V0900	01/2013-04/2022	Update of correction factors (applies to GOME-2B/-2C, and TROPOMI) and extension in time
	V1000	01/2013-10/2022	Update of correction factors (applies to GOME-2B/-2C, and TROPOMI) and extension in time
TC_MSR	V0020	04/1970-01/2018	

	V0021	01/1979-12/2018	Small bug for the longitudes, corrected in version 0021. The data of 1970-1979 have a lower resolution than the later data. Therefore, these files did not have this longitude bug. So, there is no need to update them.
	V0022	12/2018-12/2020	ERA5 used.
	V0023	04/1970-12/2018	v0020 (<1979) + v0021 (>1979) with bug fix time (changing unit attribute of time variable from months into days.)
	V0024	12/2018-12/2021	v0022 with bug fix time (changing unit attribute of time variable from months into days).
	V0025	01/2022-	V0024 with twilight chemistry correction to have an identical algorithm as used in the Ozone CCI+ project.
TC_IASI-A	V0001	10/2007-01/2020	
	V0002	02/2020-07/2020	L2 now obtained from FORLI algorithm running at Eumetsat instead of the L2 running at ULB-LATMOS.
	V0003	12/2019-08/2021	V0002 with small bug fixed in L2
06TC_IASI-A	V0001	10/2007-01/2020	
	V0002	02/2020-07/2020	L2 now obtained from FORLI algorithm running at Eumetsat instead of the L2 running at ULB-LATMOS.
	V0003	12/2019-08/2021	V0002 with small bug fixed in L2
TC_IASI-B	V0001	05/2013-01/2020	
	V0002	02/2020-07/2020	L2 now obtained from FORLI algorithm running at Eumetsat instead of the L2 running at ULB-LATMOS.
	V0003	12/2019-	V0002 with small bug fixed in L2
06TC_IASI-B	V0001	05/2013-01/2020	
	V0002	02/2020-07/2020	L2 now obtained from FORLI algorithm running at Eumetsat instead of the L2 running at ULB-LATMOS.
	V0003	12/2019-	V0002 with small bug fixed in L2
TC_IASI-C	V0001	10/2019-11/2019	
	V0003	12/2019-	L2 now obtained from FORLI algorithm running at Eumetsat instead of the L2 running at ULB-LATMOS.
06TC_IASI-C	V0001	10/2019-11/2019	

	V0003	12/2019-	L2 now obtained from FORLI algorithm running at Eumetsat instead of the L2 running at ULB-LATMOS.
NP_GOME	V0004	07/1995-05/2011	
	V0005	06/1995-06/2011	Based on RAL L2 fc0214
	V0006	06/1995-06/2011	Based on RAL L2 fc0300
NP_SCIA	V0004	08/2002-02/2011	
	V0005	08/2002-04/2012	Based on RAL L2 fc0214
	V0006	08/2002-04/2012	Based on RAL L2 fc0300
NP_GOME2A	V0004	04/2007-06/2013	
	V0005	01/2007-12/2017	Based on RAL L2 fc0300
	V0006	01/2007-08/2019	Based on RAL L2 fc0301
	V0007	09/2019-10/2020	Based on RAL L2 fv0302
NP_GOME2B	V0005	05/2013-12/2017	Based on RAL L2 fc0215
	V0006	04/2013-12/2017	Based on RAL L2 fc0300
	V0007	06/2014-11/2020	Based on RAL L2 fv0302
	V0008	11/2020-10/2021	Based on RAL L2 fv0303 and fv0305
	V0009	07/2021-06/2023	Based on RAL L2 fv0306
NP_OMI	V0004	10/2004-12/2015	
	V0005	01/2016-12/2017	Based on RAL L2 fv0214
	V0006	10/2004-08/2019	Based on RAL L2 fv0214 with filtering updates (row anomaly, etc)
	V0007	09/2019-10/2021	Based on RAL L2 fv0214 with filtering updates (row anomaly, etc)
NP_GOP-ECV	V0100	07/1995-10/2021	
LMZ_MIPAS	V0001	07/2002-04/2012	Based on Level 2 KIT v7
	V0002	07/2002-04/2012	Based on Level 2 KIT v8
LMZ_GOMOS	V0001	08/2002-12/2011	
LMZ_SCIA	V0001	08/2002 -03/2012	
LMZ_SAGE2	V0001	10/1984-08/2005	
LMZ_HALOE	V0001	10/1991-09/2005	
LMZ_SMR (*)	V0001	07/2001-08/2014	
LMZ_OSIRIS	V0001	11/2001-12/2020	Based on Level 2 USask v5.10

	V0002	11/2001-	Based on Level 2 USask v7.2
LMZ_ACE	V0001	02/2004-12/2020	Based on Level 2 v3.5/3.6
	V0002	02/2004-	Based on Level 2 v.4.1/4.2
LMZ_SABER	V0001	01/2002-07/2019	with ERA/Interim pressure-altitude information
	V0002	01/2002-	With ERA-5 pressure-altitude information
LMZ_MLS	V0001	08/2004-07/2019	Based on Level 2 NASA v4.2 with ERA-Interim
	V0002	08/2004-12/2021	Based on Level 2 NASA v4.2 with ERA-5
	V0003	08/2004-	Based on Level 2 NASA v5.0
LMZ_OMPS-SASK	V0002	02/2012-	
LMZ_OMPS-UB	V0001	02/2012-12/2021	Based on Level 2 UBr v3.4
	V0002	02/2012 -	Based on Level 2 UBr v.4.0
LMZ_SAGE-III	V0003	06/2017-	
LMZ_MERGED	V0001	10/1984-02/2017	Original SAGE-CCI-OMPS dataset
	V0002	10/1984-01/2018	extension
	V0003	10/1984-12/2018	extension
	V0004	01/2018-12/2019	extension
	V0005	10/1984-12/2019	extension
	v0006	10/1984-12/2020	extension
	V0007	10/1984-12/2021	extension + new versions of MIPAS and OSIRIS
	V0008	10/1984-12/2022	SAGE-CCI-OMPS+ dataset (latest data versions, added SAGE III/ISS, POAM III and OMPS-LP USask)
LP_MERGED	V0001	11/2001-12/2019	original dataset
	V0002	11/2001-12/2020	extension
	V0003	11/2001-12/2021	MEGRIDOP (added MLS and OMPS-LP data)
	V0004	11/2001-	extended MEGRIDOP with new versions of MIPAS and MLS

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