ECMWF COPERNICUS REPORT

Copernicus Climate Change Service

System Quality Assurance Document

Atmospheric Composition ECVs

Annex A: Ozone Products

Issue 5, Version 1.0

Issued by: BIRA-IASB / Michel Van Roozendael

Date: 29/03/2021

Ref: C3S_312b_Lot2.2.0-v5_SQAD_202103_Annex_A_Ozone_v1.0

Official reference number service contract: 2018/C3S_312b_Lot2_DLR/SC1

IMPLEMENTED BY ECMWF

Contributors

BIRA-IASB
M. Van Roozendael
A. De Rudder
C. Lerot
J. Vlietinck
A. Keppens
D. Hubert
T. Verhoelst
J.-C. Lambert

LATMOS/UPMC
A. Boynard
C. Clerbaux

DLR
D. Loyola
K.-P. Heue
M. Coldewey-Egbers

UiB
K.-U. Eichmann
M. Weber

KNMI
R. van der A
M. van Weele
J. van Peet
O. Tuinder
M. Allaart

RAL
B. Latter
R. Siddans
B. Kerridge

FMI
V. Sofieva
J. Tamminen

History of modifications

Version	Date	Description of modification	Chapters / Sections
Issue 1			
v1	26/03/2019	Update of the C3S_312a_Lot4 Ozone SQAD and harmonisation with the GHG SQAD	all
v1.1	21/5/2019	Minor corrections as suggested by ASSIMILA	
Issue 2			
	30/09/2019	Re-issued without change	
Issue 3			
v1.0	24.03.2020	Re-issued without change	
Issue 4			
v1.0	03.10.2020	Update about SMR	List of datasets covered (SMR) General definitions (L3 data) System overview (Fig 1) Table 1: SMR
Issue 5			
v1.0	29.03.2021	General update	all

List of datasets covered by this document

Deliverable ID	Product title	Product brief description	Delivery number	Due delivery date
ICDR quarterly extensions			1.1	28/02/2019
D312b_Lot2.3.3.1.1	TC_GOME2A	GOME-2A / total column L3 ICDR	1.2	31/05/2019
D312b_Lot2.3.3.1.2	TC_GOME2B	GOME-2B / total column L3 ICDR	1.3	31/08/2019
D312b_Lot2.3.3.1.3	TC_OMI	OMI / total column L3 ICDR	1.4	30/11/2019
D312b_Lot2.3.3.1.4	TC_OMPS	OMPS / total column L3 ICDR	1.5	28/02/2020
D312b_Lot2.3.3.1.5	TC_IASI-A	IASI-A / total column L3 ICDR	1.6	31/05/2020
	TC_IASI-B	IASI-B / total column L3 ICDR	1.7	31/08/2020
	06TC_IASI-A	IASI-A / tropospheric column L3 ICDR	1.8	30/11/2020
	06TC_IASI-B	IASI-B / tropospheric column L3 ICDR	1.9	28/02/2021
ICDR half-yearly extensions			1.1	28/02/2019
D312b_Lot2.3.3.1.6	TC_GTO-ECV	GTO merged / total column L3 ICDR	1.2	31/08/2019
			1.3	28/02/2020
			1.4	31/08/2020
			1.5	28/02/2021
ICDR yearly extensions			1.1	28/02/2019
D312b_Lot2.3.3.1.7	TC_MSR	Multi-sensor assimilated total column L4 ICDR	1.2	28/02/2020
D312b_Lot2.3.3.1.8	NP_GOME2A	GOME-2A nadir profile L3 ICDR	1.3	28/02/2021
D312b_Lot2.3.3.1.9	NP_GOME2B	GOME-2B nadir profile L3 ICDR		
D312b_Lot2.3.3.1.10	NP_OMI	OMI nadir profile L3 ICDR		
D312b_Lot2.3.3.1.11	LMZ_OSIRIS	OSIRIS limb profiles L3 ICDR		
D312b_Lot2.3.3.1.12	LMZ_OMPS	OMPS limb profiles L3 ICDR		

Deliverable ID	Product title	Product brief description	Delivery number	Due delivery date
D312b_Lot2.3.3.1.13	LMZ_ACE	ACE limb profiles L3 ICDR		
D312b_Lot2.3.3.1.14	LMZ_MLS	MLS limb profiles L3 ICDR		
D312b_Lot2.3.3.1.15	LMZ_SABER	SABER limb profiles L3 ICDR		
D312b_Lot2.3.3.1.16	LMZ_MERGED	Merged zonal mean limb profiles L3 ICDR		
D312b_Lot2.3.3.1.17	LP_MERGED	Merged gridded limb profiles L3 ICDR		
Complete CDR time series			2.0	28/02/2021
D312b_Lot2.3.3.1.18	TC_GOME	GOME / total column L3 CDR (06.1995 – 07.2011)		
D312b_Lot2.3.3.1.19	TC_SCIA	SCIAMACHY / total column L3 CDR (08.2002 – 04.2012)		
D312b_Lot2.3.3.1.20	NP_GOME	GOME / nadir profiles L3 CDR (06.1995 – 06.2011)		
D312b_Lot2.3.3.1.21	NP_SCIA	SCIAMACHY / nadir profiles L3 CDR (08.2002 – 04.2012)		
D312b_Lot2.3.3.1.22	LMZ_MIPAS	MIPAS / limb profiles L3 CDR (07.2002 – 04.2012)		
D312b_Lot2.3.3.1.23	LMZ_GOMOS	GOMOS / limb profiles L3 CDR (08.2002 – 12.2011)		
D312b_Lot2.3.3.1.24	LMZ_SCIA	SCIAMACHY / limb profiles L3 CDR (08.2002 – 03.2012)		
D312b_Lot2.3.3.1.25	LMZ_SAGE2	SAGE-2 / limb profiles L3 CDR (10.1984 – 08.2005)		
D312b_Lot2.3.3.1.26	LMZ_HALOE	HALOE / limb profiles L3 CDR (10.1991 – 09.2005)		
No deliverable ID	LMZ_SMR	SMR / limb profiles L3 CDR (07.2001 – 08.2014) [1]		

Related documents

Reference ID	Document
D1	**ESA-CCI-O3-SSDv1.2:** Wolfmüller, M., 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 System Specification Document (SSD), Ozone_cci_DLR_SS_01_02, May 15, 2017.
D2	**ESA-CCI-O3-SVRv2:** Wolfmüller, M., 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 and M. Weber, Ozone_cci System Verification Report (SVR), Ozone_cci_DLR_SVR_02, May 15, 2017.
D3	**C3S-312a-O3-FAQ 2018:** C3S Ozone CDR FAQ, June 6, 2018.
D4	**C3S-312a-O3-PQARv2:** Hubert, D., A. Keppens, T. Verhoelst, J. Granville and J.-C. Lambert, C3S 312a Lot4 Product Quality Assessment Report (PQAR), Version 2, C3S_312a_Lot4.3.2.3-3.2.8_201807_PQAR_v2, 51 pp., July 31, 2018.

[1] SMR is still in operation but the L1 data processing has been interrupted, which is why the L2/L3 record currently stops in August 2014. It may resume later, since the reprocessing of the Odin entire data record is underway at Chalmers University and *soon to be closed* (https://odin.rss.chalmers.se/#documents). Under C3S 312b Lot2, it is currently being delivered to the C3S Climate Data Store (CDS) as a completed CDR (July 2001 – August 2014, with one missing month: September 2001).

Reference ID	Document
D5	**C3S-312b-O3-TRGAD-2020:** Van Roozendael, M. (ed.) and the C3S Ozone team, C3S 312b Lot2 Ozone Target Requirements and Gap Analysis Document (TRGAD), Version 3.0, C3S_312b_Lot2.1.0-2020(O3)_TRD-GAD_v3.0, December 9, 2020.
D6	**C3S-312a-O3-SQADv2:** Van Roozendael, M., A. De Rudder, C. Lerot, J. Vlietinck, A. Keppens, D. Hubert, J.-C. Lambert, A. Boynard, C. Clerbaux, D. Loyola, K.-P. Heue, M. Coldewey-Egbers, N. Rahpoe, K.-U. Eichmann, M. Weber, R. van der A, M. van Weele, J. van Peet, M. Allaart, B. Latter, R. Siddans, B. Kerridge, V. Sofieva, S. Tukiainen, J. Tamminen, F. Done, R. Mannan, S. O'Hara and R. Cifres, C3S 312a Lot4 System Quality Assurance Document (SQAD), Versions 1 and 2, C3S_312a_Lot4.3.1.10-15_201804_SQAD_v1_v2, 59 pp., February 7, 2019.
D7	**C3S-312b-O3-ATBDv2.0:** Van Roozendael, M. (ed.) and the C3S Ozone team, C3S 312b Lot2 Ozone Algorithm Theoretical Basis Document (ATBD), Version 2.0, C3S_312b_Lot2.1.1.2_202102_ATBD_v2.0, March 25, 2021.
D8	**C3S-312b-O3-PUGSv2.0:** Van Roozendael, M. (ed.) and the C3S Ozone team, C3S 312b Lot2 Ozone Product User Guide and Specification (PUGS), Version 2.0, C3S_312b_Lot2.3.2.1_202102_PUGS_O3_v2.0, March 25, 2021.
D9	**C3S-312b-O3-PQADv2.0:** Hubert, D., A. Keppens, T. Verhoelst, J. Granville and J.-C. Lambert, C3S 312b Lot2 Ozone Product Quality Assurance Document (PQAD), Version 2.0, C3S_D312b_Lot2.2.1.1_202102_PQAD_O3_v2.0, February 28, 2021.
D10	**C3S-312a-O3-FR:** Van Roozendael, M., A. De Rudder, C. Lerot, J. Vlietinck, A. Keppens, D. Hubert, J.-C. Lambert, A. Boynard, C. Clerbaux, D. Loyola, K.-P. Heue, M. Coldewey-Egbers, N. Rahpoe, K.-U. Eichmann, M. Weber, R. van der A, M. van Weele, J. van Peet, M. Allaart, B. Latter, R. Siddans, B. Kerridge, V. Sofieva, S. Tukiainen, J. Tamminen, F. Done, R. Mannan, S. O'Hara and R. Cifres, C3S 312a Lot4 Final Report (FR), C3S_ D312a_Lot4.0.1.11_201812_Final_Report_v1, March 25, 2019.

Acronyms

Acronym	Definition
AATSR	Advanced Along-Track Scanning Radiometer
ACCENT	Atmospheric Composition Change: the European Network (EU FP7 network of excellence)
ACE	Atmospheric Chemistry Experiment
AC SAF	SAF for Atmospheric Composition Monitoring (Eumetsat)
ALGOM	GOMOS Level2 Algorithm Evolution Studies (ESA-funded project)
AUTH	Aristotle University of Thessaloniki
BESD	Bremen Optimal Estimation DOAS
BIRA-IASB	Royal Belgian Institute for Space Aeronomy
BUV	Backscattered Ultraviolet
CAMS	Copernicus Atmosphere Monitoring Service

Acronym	Definition
CCI	Climate Change Initiative (ESA)
CDOP	Continuous Development and Operations Phase (of O3M SAF)
CDR	Climate Data Record
CDS	Climate Data Store
CEDA	Centre for Environmental Data Analysis (UK)
CEMS	Climate and Environmental Monitoring from Space
CEOS	Committee on Earth Observation Satellites
CETP	Centre des Environnements Terrestres et Planétaires
CHEOPS-GOME	Climatology of Height-resolved Earth Ozone and Profiling Systems for GOME
CHEOPS-SCIA	Climatology of Height-resolved Earth Ozone and Profiling Systems for SCIAMACHY
CityZen	megaCITY - Zoom for the Environment (EU FP7 project)
CMA	China Meteorological Administration
CMS	Content Management System
CNES	Centre National d'Études Spatiales (French Space Agency)
CNRS	Centre National de la Recherche Scientifique
CPU	Central Processing Unit
CSA	Canadian Space Agency
CSV	Comma-Separated Values format
CUS	Copernicus User Support
C3S	Copernicus Climate Change Service
DEM	Digital Elevation Model
DFD	German Remote Sensing Data Centre (DLR)
DISORT	Discrete-Ordinate-Method Radiative Transfer (Fortran program)
DLR	Deutsches Zentrum für Luft- und Raumfahrt (German Aerospace Centre)
DOAS	Differential Optical Absorption Spectroscopy
DoD	Department of Defense (USA)
ECCC	Environment and Climate Change Canada
ECMWF	European Centre for Medium-Range Weather Forecasts
ECSTRA	Extinction Coefficient for STRatospheric Aerosol
ECV	Essential Climate Variable
Envisat	Environmental Satellite (ESA)
EOC	Earth Observation Centre (DLR)
EOS	Earth Observing System
EP	Earth Probe
EPS	Eumetsat Polar System
EPS-SG	EPS Second Generation
EQC	Evaluation and Quality Control
ERA	ECMWF Re-Analysis
ERBS	Earth Radiation Budget Satellite
ERS	European Remote-Sensing Satellite

Acronym	Definition
ESA	European Space Agency
EU	European Union
EUMETSAT	European Organisation for the Exploitation of Meteorological Satellites
EVOSS	European Volcano Observatory Space Services (EU FP7 project)
FAQ	Frequently Asked Question
FMI	Finnish Meteorological Institute
FMI-EO	FMI Earth Observation unit
FORLI	Fast Optimal/Operational Retrieval on Layers for IASI
FTIR	Fourier-Transform Infra-Red spectroscopy
FP5	Fifth Framework Programme (EU)
FP6	Sixth Framework Programme (EU)
FP7	Seventh Framework Programme (EU)
FTP	File Transfer Protocol
FY	Feng Yun (Chinese satellite)
GAIA-CLIM	Gap Analysis for Integrated Atmospheric ECV Climate Monitoring (EU H2020 project)
GCOS	Global Climate Observing System
GDP	GOME Data Processor
GEOMon	Global Earth Observation and Monitoring (EU FP6 project)
GHG	Greenhouse Gas(es)
GISS	Goddard Institute for Space Studies
GMES	Global Monitoring for Environment and Security (ESA)
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 and Metop-B)
GOMOS	Global Ozone Monitoring by Occultation of Stars
GOSAT	Greenhouse Gases Observing Satellite (JAXA)
GSE	GMES Service Element (ESA)
GSFC	Goddard Space Flight Center
GTO	GOME-type Total Ozone
HA	High Availability
HALOE	Halogen Occultation Experiment
HGF	Helmholtz-Gemeinschaft der Forschungszentren
HLRN	Norddeutscher Verbund für Hoch- und Höchstleistungsrechnen (North-German Supercomputing Alliance)
HPC	High Performance Computing/Computer
HQ	Headquarters
HYMN	Hydrogen, Methane and Nitrous oxide: Trend Variability, Budgets and Interactions with the Biosphere (EU FP6 project)
H2020	Horizon 2020 (EU research and development programme)
IASB-BIRA	Royal Belgian Institute for Space Aeronomy

Acronym	Definition
IASI	Infrared Atmospheric Sounding Interferometer
IASI-NG	IASI New Generation
ICDR	Intermediate Climate Data Record
ICT	Information and Communication Technology/Technologies
IDL	Interactive Data Language
IEA	Institute for Environmental Analytics (UK)
IMF	Remote Sensing Technology Institute (DLR)
IPSL	Institut Pierre Simon Laplace
IR	Infra-Red
IUP-UB	Institute of Environmental Physics, University of Bremen
JAXA	Japan Aerospace Exploration Agency
KIT	Karlsruhe Institute of Technology
KNMI	Royal Netherlands Meteorological Institute
KPI	Key Performance Indicator
LAN	Local Area Network
LATMOS	Laboratoire Atmosphères et Observations Spatiales
LP	Limb Profile/Profiler
LUT	Look-Up Table
L1	Satellite Data Processing Level 1
L2	Satellite Data Processing Level 2
L3	Satellite Data Processing Level 3
L4	Satellite Data Processing Level 4
MACC	Monitoring Atmospheric Composition and Climate (EU FP7 project)
MERIS	Medium Resolution Imaging Spectrometer (ESA Envisat)
MesosphEO	Exploitation of the Mesosphere (ESA-funded project)
Metop	Meteorological Operational Platform (EUMETSAT)
MIPAS	Michelson Interferometer for Passive Atmospheric Sounding
MLER	Minimum Lambertian Equivalent Reflectivity
MLS	Microwave Limb Sounder
MLT	Mid and Lower Troposphere
MPC	Mission Performance Centre
MSG	Meteosat Second Generation (Eumetsat)
MSR	Multi-Sensor Reanalysis
Multi-TASTE	Multi-Mission Technical Assistance to Envisat and TPMS Validation by Sondes, Spectrometers and Radiometers
MW	Microwave
NASA	National Aeronautics and Space Administration (USA)
NCEO	National Centre for Earth Observation (UK)
NDACC	Network for the Detection of Atmospheric Composition Change
NERC	Natural Environment Research Council (UK)
NetCDF	Network Common Data Form (data file format)

Acronym	Definition
NLC	Noctilucent Cloud
NOAA	National Oceanic and Atmospheric Administration (USA)
NP	Nadir Profile
NRC	National Research Council
NRSCC	National Remote Sensing Center of China
OMI	Ozone Monitoring Instrument (aboard EOS-Aura)
OMPS	Ozone Mapping and Profiler Suite
ORAC	Oxford-RAL Aerosol and Cloud retrieval scheme
OSIRIS	Optical Spectrograph and InfraRed Imaging System (aboard Odin)
Ozone_cci	ESA Climate Change Initiative ozone project
O3M SAF	SAF for Atmospheric Composition and UV Radiation (Eumetsat) – replaced by AC SAF
PA	Institut für Physik der Atmosphäre (DLR)
PANDA	Partnership with China on Space Data (EU FP7 project)
PASODOBLE	Promote Air Quality Services integrating Observations – Development Of Basic Localised Information for Europe (EU FP7 project)
PB	Petabyte
PI	Principal Investigator
POET	Precursors of Ozone and their Effects in the Troposphere (EU FP5 project)
PROMOTE	PROtocol MOniToring for the GMES Service Element: Atmosphere
PSC	Polar Stratospheric Cloud
PUGS	Product User Guide and Specification
QA4ECV	Quality Assurance for Essential Climate Variables (EU FP7 project)
RAL	Rutherford Appleton Laboratory
RAM	Random Access Memory
RCS	Revision Control System (version management software)
RD	Research and Development
RMI	Royal Meteorological Institute of Belgium
ROB	Royal Observatory of Belgium
RSG	Remote Sensing Group (at RAL)
RTTOV	Radiative Transfer for TOVS (radiative transfer model)
R&D	Research and Development
SA	Service d'Aéronomie
SABER	Sounding of the Atmosphere using Broadband Emission Radiometry
SAF	Satellite Application Facility
SAGE	Stratospheric Aerosol and Gas Experiment
SBUV	Solar Backscatter Ultraviolet Radiometer
SCIAMACHY	Scanning Imaging Absorption Spectrometer for Atmospheric CHartographY (aboard Envisat)
SECTEUR	Sector Engagement for C3S: Translating European User Requirements
SHADOZ	Southern Hemisphere Additional Ozonesonde Network

Acronym	Definition
SHDOM	Spherical Harmonic Discrete Ordinate Method (to compute atmospheric radiative transfer)
SIS	Sectorial Information Service (C3S)
SMR	Sub-Millimetre Radiometer (aboard Odin)
SNSB	Swedish National Space Board
SQAD	System Quality Assurance Document
SVN	Subversion (version management software)
S5P	Sentinel-5 Precursor (ESA satellite)
TASTE	Technical ASsistance To Envisat
TC	Total Column
TCDR	Thematic Climate Data Record
TEMIS	Tropospheric Emission Monitoring Internet Service
TIROS	Television Infrared Observation Satellite(s) (NASA)
TOC	Total Ozone Column
TOMS	Total Ozone Mapping Spectrometer
TOU	Total Ozone Unit
TOVS	TIROS Operational Vertical Sounder (aboard TIROS)
TROPOMI	Tropospheric Monitoring Instrument (on board S5P)
TVUK	Telespazio VEGA UK
UARS	Upper Atmosphere Research Satellite
UK	United Kingdom
ULB	Université Libre de Bruxelles
UMR	Unité Mixte de Recherche
UNEP	United Nations Environmental Programme
UNFCCC	United Nations Framework Convention on Climate Change
UNI-HB	University of Bremen
UPMC	University Pierre et Marie Curie
USA	United States of America
USGS	United States Geological Survey
UTLS	Upper Troposphere / Lower Stratosphere
UV	Ultraviolet
UVN	Ultra-Violet/Visible/Near-Infrared
UVSQ	University Versailles Saint-Quentin en Yvelines
VDAF	Validation Data Analysis Facility
VIIRS	Visible Infrared Imaging Radiometer Suite
WAN	Wide Area Network
WFDOAS	Weighting Function Differential Optical Absorption Spectroscopy
WISC	Wind Storm Information Service (C3S SIS project)
WMO	World Meteorological Organization
WOUDC	World Ozone and Ultraviolet Radiation Data Centre (at ECCC) http://www.woudc.org/

Acronym	Definition
WP	Work Package
3MI	Multi-viewing Multi-channel Multi-polarization Imaging

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)*.

Fundamental climate data record (FCDR)

A fundamental climate data record (FCDR) is a CDR of calibrated and quality-controlled data designed to allow the generation of homogeneous products that are accurate and stable enough for climate monitoring.

Thematic climate data record (TCDR)

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

Intermediate climate data record (ICDR)

An intermediate climate data record (ICDR) is a TCDR which undergoes regular and consistent updates *(Werscheck, 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 *(Parkinson et al., 2006)*.

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. ozone column) 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)

The C3S ozone data products include the following types of data.

- Level 3 data:
  - gridded monthly averages covering the globe;
  - monthly zonal averages over 10° latitude bands (ozone profiles from individual limb instruments and LMZ_MERGED merged dataset).
- Level 4 data:
  - gridded monthly averaged assimilated ozone total column (TC_MSR).

Table of Contents

Scope of the document

This document is the C3S Ozone System Quality Assurance Document (SQAD). It describes all elements that contribute to the processing chain, including all interfaces to C3S and to R&D components, the hardware used in the processing chain, the procedures to implement new data cycles and to reprocess the products, and those applied in case of system failures or anticipated maintenance work, as well as information on user support.

The system specifications are derived from specifications established as part of the heritage ESA Climate Change Initiative ozone project (Ozone_cci). The processing system consists in a decoupled and fully distributed system spread over several organisations where each contributor provides existing systems for the generation of the committed ozone data sets.

Based on this architecture, the following L3 and L4 ECV parameters are generated:

- total ozone from UV nadir instruments;
- total and tropospheric ozone column from the IASI sensor;
- low vertical resolution ozone profiles from nadir UV sensors;
- stratospheric and upper tropospheric ozone profiles from limb and occultation sensors.

The Ozone ECV products are generated using the following L1 and L2 data sets:

- input data from GOME, SCIAMACHY, GOME-2A, GOME-2B, OMI, OMPS for total ozone, plus data from BUV-Nimbus4, TOMS-Nimbus7, TOMS-EP, SBUV-7, -9, -11, -14, -16, -17, -18 and -19, OMPS and TOU-FY3A/B for the total ozone multi-sensor reanalysis (MSR);
- input data from IASI for total and tropospheric ozone columns from IASI;
- input data from GOME, SCIAMACHY, GOME-2A/B, OMI for ozone nadir profiles;
- input data from MIPAS, GOMOS, SCIAMACHY, SAGE-2, HALOE, SMR[2], OSIRIS, OMPS-LP, ACE, MLS, SABER for the generation of ozone limb and occultation profiles.

Executive summary

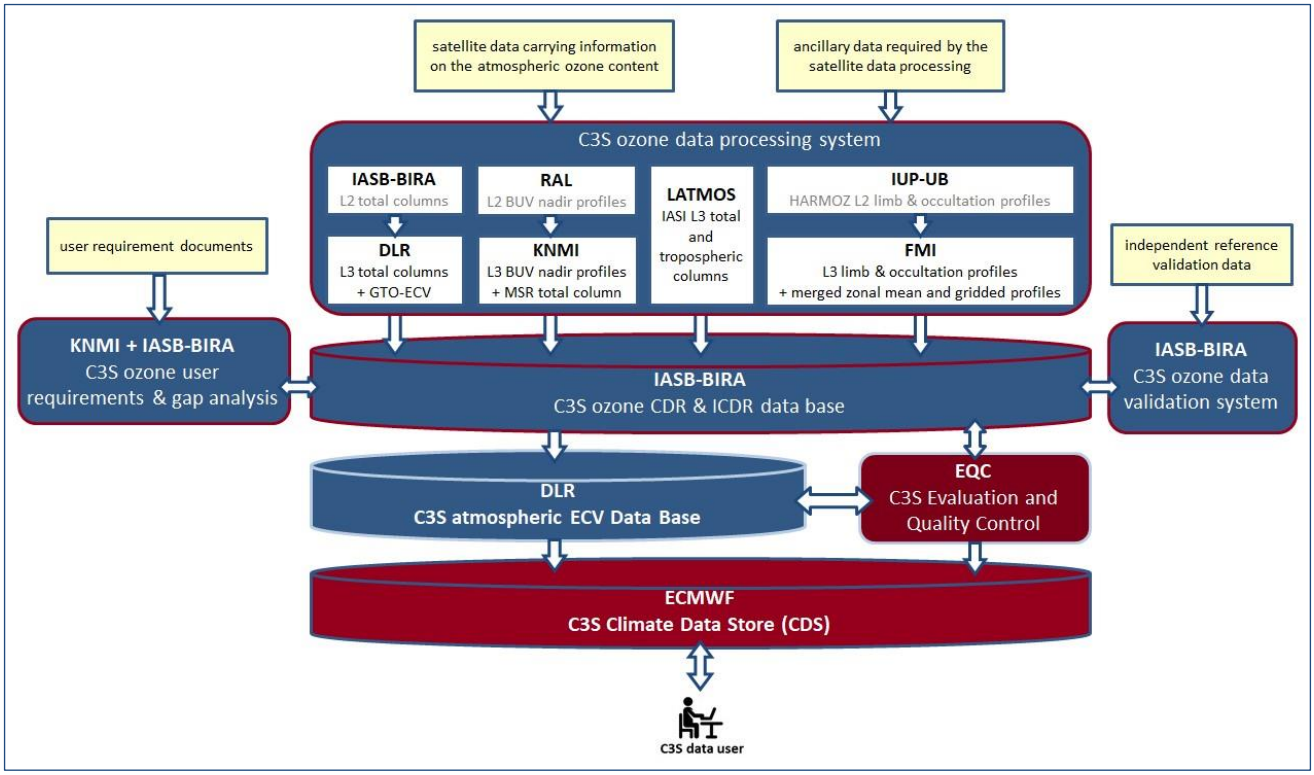
This issue of the C3S Ozone System Quality Assurance Document (SQAD) covers the implementation cycles of the ozone data release under Contract C3S_312b_Lot2, including data processing, validation and delivery to the DLR C3S database. The different components of the system and its internal and external interfaces are described in Section 1. ICDR are regularly expanded with the most recent observations. Section 2 provides details on the scheduled regular data upgrades. Section 3 gives information on the conditions determining data reprocessing (e.g. retrieval algorithm upgrade, instrumental drift correction, …) and Section 4 on the controls in place to cope with accidental failure of each part of the system. Section 5 addresses user support.

[2] Under discussion at the time of writing.

1. System overview

A schematic picture of the C3S ozone data production system is provided in **Fehler! Verweisquelle konnte nicht gefunden werden.**. Its different elements and interfaces are described in the next subsections.

Figure 1 – Schematic picture of the C3S ozone system (in blue) and its internal and external interfaces.



1.1 System elements and interfaces

1.1.1 C3S ozone teams

The teams involved in generating the C3S ozone datasets are described below. Their respective roles in the C3S ozone data production system are described in Sections 1.1.4 (P. 28) to 1.1.7 (P. 31).

1.1.1.1 Royal Belgian Institute for Space Aeronomy (IASB-BIRA)

BIRA-IASB is a federal research institute mandated to carry out scientific research and deliver public services in the field of aeronomy. Since its foundation, BIRA-IASB has developed an internationally acknowledged expertise in numerical modelling and measurements of the atmospheric composition. Its focus also extends to the atmosphere of other planets, and of outer space. BIRA-IASB has a strong expertise in designing and operating instruments and experiments to monitor atmospheres and space environment. It has also developed a strong know-how in the exploitation of measurements from

ground, air and space, as well as their geophysical interpretation using, among others, theoretical and numerical models.

One of the main topics of interest at BIRA-IASB is the study and the monitoring of the ozone layer in the Earth stratosphere and related key parameters like polar stratospheric clouds, halogenated compounds, reactive gases and stratospheric aerosols. BIRA-IASB contributes to the evaluation of long-term changes of atmospheric ozone concentrations. Forecasting capabilities have also been developed based on chemical transport models. Important research activities are also dedicated to the Earth tropospheric chemistry, with a focus on natural and manmade emissions, like SO_2 and NO_2, tropospheric ozone precursors and their relationship with air quality issues. In relation with the global warming, BIRA-IASB contributes to the monitoring of the evolution of atmospheric greenhouse gases concentrations in support of the Kyoto Protocol. Forecasting of chemical weather is being developed.

Since the launch of ERS-2 GOME in 1995, BIRA-IASB has been strongly involved in the exploitation of the successive GOME, SCIAMACHY, GOME-2 and OMI missions through retrieval algorithm development and various contributions to the geophysical data validation. The institute also plays a leading role in the international Network for the Detection of Atmospheric Composition Change (NDACC), being a co-chair of its steering committee as well as a co-chair of its UV-Vis and Satellite working groups.

Within the successive ESA GODFIT, GDP4, GDP5 and Ozone_cci projects, BIRA-IASB scientists have developed an acknowledged expertise with total ozone retrieval. As part of the Ozone_cci project which is led by BIRA-IASB, the institute is responsible for the generation of the level-2 total ozone data products from the GOME, SCIAMACHY, GOME-2, OMI and OMPS sensors, all of them being processed using a harmonised retrieval baseline. This is performed in close collaboration with DLR-IMF, RT-Solutions Inc. and AUTH. In the same project, BIRA-IASB also coordinates the geophysical validation of all ozone data products. Over the last decade, BIRA-IASB has been involved in many EU, ESA and EUMETSAT projects. In particular it has been closely associated to the management and activities of GSE PROMOTE and PROMOTE Stage 2 projects. Within Copernicus/GMES, it has also been involved in the EU FP7 MACC-1/2/3, PASODOBLE and EVOSS projects. BIRA-IASB is part of all Envisat Quality Working Groups, and is Lead of the Multi-TASTE, TASTE-F and CEOS inter-calibration projects.

BIRA-IASB has been Science Leader of the ESA Ozone_cci project and is Science Leader of its Ozone_cci+ follow-up, where it is responsible for total ozone level-2 algorithm development and data processing as well as for the coordination of the validation tasks of all ozone data products. It is also involved in a number of related projects, most of them under ESA funding or through joint national-ESA funding. In the context of the preparation of the Sentinel 4, 5 and 5P missions, BIRA-IASB is in charge of the definition of prototype level-2 retrieval algorithms for total ozone, formaldehyde, SO_2 and glyoxal products. As part of the Sentinel-5 Precursor Mission Performance Center (MPC), it is also responsible for the operational validation system (VDAF) which is being developed and operated on-site. The expertise of BIRA-IASB in atmospheric composition monitoring from space and its synergies with ground-based networks has been built through participation to a large number of projects started in the late nineties. In particular BIRA-IASB has been involved in the successive TEMIS, GSE PROMOTE, GEOmon, GODFIT, GDP4 and GDP5 projects. It has also been part of the CHEOPS-GOME and CHEOPS-SCIA nadir ozone profiling developments, and the SCIAMACHY and MIPAS Quality Working Groups. Since the launch of the MetOp-A platform in 2006, it has been involved in the activities of the EUMETSAT O3M-SAF supporting data product developments in cooperation with DLR

and being in charge of trace gas validation activities. BIRA has also participated to several EU projects pioneering the future Copernicus Climate Change Service (C3S), in particular the FP7 QA4ECV and H2020 GAIA-CLIM projects which both deal with establishing improved frameworks for ECV data quality assessment and identification of gaps in measurements and uncertainty characterisation.

BIRA-IASB was the main contractor of the C3S_312a_Lot4 contract with ECMWF (November 2016 – October 2018) to deliver the initial versions of the C3S ozone data products to the CDS [D10].

1.1.1.2 German Aerospace Centre (DLR)

The Deutsches Zentrum für Luft- und Raumfahrt e.V. (DLR) is the German national research establishment for aeronautics, astronautics, and energy technology. DLR is a large research centre within the Helmholtz-Gemeinschaft der Forschungszentren (HGF). DLR is responsible for the management of the German national space programme.

The Remote Sensing Technology Institute of DLR (DLR-IMF) carries out research and development of remote sensing technologies with an emphasis on methodologies, techniques and processing systems for retrieval of information from remote sensing data and archives. The processors it develops function operationally to the largest extent possible so they can be integrated in EOC processing chains. IMF operates an airborne optical sensor suite, a calibration and spectrometry laboratories furnishing the basis for the best possible use of remote sensing data. In addition, IMF contributes to the design of new sensor systems and earth observation systems and pursues technology transfer. DLR-IMF has over 17 years of experience on operational trace gas retrieval algorithms and systems and is responsible for the generations of the operational GOME, SCIAMACHY and GOME-2 products on behalf ESA and EUMETSAT. DLR-IMF together with the partner organizations BIRA, RTS Inc and AUTH develop the GDP algorithms for the operational ozone total column retrieval.

The Remote Sensing Technology Institute (IMF), the Institut für Physik der Atmosphäre (PA) and the German Remote Sensing Data Center (DFD) are all located at Oberpfaffenhofen. IMF and DFD comprise the DLR's Earth Observation Center (EOC) engaged in research, product development/generation and providing services based on earth observation data from aircraft and satellite platforms.

DLR is actively involved in the ESA CCI Ozone and in the EUMETSAT O3M-SAF projects. In Ozone_cci DLR is responsible for the generation of harmonised level-3 data products of total ozone (GTO-ECV) and of tropical tropospheric ozone columns from the GOME, SCIAMACHY, GOME-2 and OMI sensors.

In the EUMETSAT O3M-SAF, DLR develops algorithms and produces operationally atmospheric trace gas data products from the GOME-2 sensors on board of the satellites MetOp-A and MetOp-B. The data encompass near real time and offline products for total and tropospheric O_3, NO_2, SO_2, BrO, HCHO, H_2O, OClO and glyoxal.

1.1.1.3 Rutherford Appleton Laboratory (RAL)

The RAL Remote Sensing Group (RSG) produces global data sets on ozone, methane, aerosol and cloud from satellite instruments. Other areas of activity include development and application of radiative transfer and retrieval models to simulate future instrument capabilities, data analysis and scientific interpretation. These activities specifically encompass UV/visible/IR spectrometry, and

analysis of multi-spectral imager data for cloud and aerosol, using optimal estimation theory. RSG has a long-standing involvement in the UK National Centre for Earth Observation (NCEO). The RSG is currently involved in ESA CCI projects on ozone, aerosol and cloud to provide multi-year, self-consistent data sets, requiring extensive consideration of changes in instrument performance during their lifetime as well as an understanding of the different instrument characteristics. Members of the group are involved in Science / Mission Advisory Groups for GOME, SCIAMACHY, AATSR, 3MI and Sentinel 4/5.

RAL has been participating in a number of related projects funded nationally and by ESA.

Most of the scientific retrieval algorithm development at RAL, notably including the UV O_3 profiling scheme, IASI methane scheme and cloud and aerosol schemes have been supported by the National Centre for Earth Observation – UK NERC Research Centre. RAL is also strongly involved in the ESA Ozone_cci project where it is responsible for developing the algorithm to provide O_3 profiles from nadir sensors, as well as performing the related full mission data processing (GOME-1, SCIAMACHY, GOME-2A and -2B and OMI).

Another important related activity is being developed in the ESA Sentinel-5 Precursor Level 2 development project where RAL is responsible for O_3 profile verification and development of the operational code to provide cloud and radiance information from the VIIRS imager for use in other S5P L2 algorithms. RAL also contributes to the Consolidation of Requirements for the Sentinel 5 UVN Band (ESA study) through retrieval simulations to consolidate S5 requirements with respect to height resolved O_3 retrieval. Finally as part of the Sentinel 4 UVN Support Studies (ESA), it provides Science Support to Instrument Development for Sentinel-4. This includes spectral calibration algorithm, retrieval studies on S4 Level 2 products and investigations on mitigating impact of inhomogeneous slit filling.

1.1.1.4 Royal Netherlands Meteorological Institute (KNMI)

The Royal Netherlands Meteorological Institute is a government agency operating under the responsibility of the Ministry of Transport. It is an operational institute that provides weather observations, weather forecasts and vital weather information all year round, 24 hours a day, and 7 days a week. The institute carries out applied and fundamental research in support of its operational tasks and as a global change research centre. The institute has three main departments: Weather, Climate and Seismology, and Infrastructure. It employs approximately 400 permanent staff.

As an operational meteorological data centre and research institute in one, KNMI combines international contacts and co-operation projects in a practical sense. KNMI is an active member of such large international organisations as the World Meteorological Organisation, the European Centre for Medium-range Weather Forecasts and the European Organisation for the Exploitation of Meteorological Satellites.

Remote sensing is of great importance to the KNMI. For weather forecasting and for research and development activities satellite observations provide a valuable complement to in-situ measurements. These data are applied in the first place for KNMI's own operational meteorological and research tasks but KNMI also provides earth observation products and related services as an aid to the exertion of public tasks. Furthermore, data and value added products are provided for national and international environment and climate change programmes. KNMI is involved in national and

international studies concerning user aspects of earth observation data. KNMI aims at establishing and extending the nation-wide and European infrastructure.

The department R&D Satellite Observations contributes to research and monitoring of the Earth system by utilizing satellites. Its research activities focus on the quality and availability of satellite observations of essential atmospheric quantities for weather and climate research. The specific fields of expertise are: air quality, greenhouse gases, stratospheric ozone, clouds, aerosols, and winds. The satellite activities of the department encompass the entire range from collecting user requirements, developing and generating the required satellite products, calibration and validation of the data, to delivering products to users.

The department is the Principal investigator of the OMI and TROPOMI satellite instruments, aimed at monitoring atmospheric composition. From the satellite observations data services are being developed, aimed at weather forecasting, climate modelling, health, and safety (e.g. volcanic eruptions). Data products are provided via www.temis.nl.

KNMI is involved in the Ozone_cci, where it is responsible for the delivery of user requirements, level 3 and level 4 data products of nadir ozone profile observations. KNMI is also making a major contribution to Copernicus, both concerning the satellite infrastructure (OMI, TROPOMI) and the Copernicus Atmosphere Monitoring Service (CAMS). KNMI (Henk Eskes) is coordinating the validation project of CAMS. Other relevant projects coordinated by KNMI are QA4ECV (lead Folkert Boersma) and MarcoPolo (lead by Ronald van der A). KNMI contributes to ESA's ozone, aerosol and cloud CCI projects. Apart from this there are many contributions to other H2020 research projects.

1.1.1.5 Laboratoire Atmosphères et Observations Spatiales (LATMOS)

LATMOS (UMR 8190) is a French public laboratory associated with the Centre National de la Recherche Scientifique (CNRS), University Versailles Saint-Quentin en Yvelines (UVSQ) and University Pierre et Marie Curie-Paris (UPMC-Paris 6). LATMOS employs 250 people including about 70 permanent scientists.

LATMOS is a relatively new laboratory created on 1st January 2009 from the fusion between Service d'Aéronomie (SA) and half of the Centre des Environnements Terrestres et Planétaires (CETP). The primary objective of LATMOS is the study of physical/chemical and dynamical processes in :

- the terrestrial atmosphere and surface (particularly stratospheric ozone, oxidisation properties of the troposphere, dynamical micro-physical and radiative processes in the atmosphere, Sun-Earth interactions and climate-environment relationships);
- planetary and cometary atmospheres;
- the local interstellar and interplanetary medium.

The TROPO department inside LATMOS has been heavily involved in the conception of satellite missions, with contributions on the definition of several instruments (interactions with industry and spatial agencies), on the development of processing algorithms and on scientific exploitation of millions of measurements. The department is working with the French Spatial Agency CNES (IASI, IASI-NG, Merlin, etc.), with the European Space Agency (several concepts of missions submitted to the ESA AO), and with Eumetsat (Sentinel 4/Meteosat Third Generation and Sentinel 5/EPS-SG missions).

LATMOS researchers have been continuously involved in the WMO Ozone Assessment (WMO/UNEP) reports as Lead Authors, Contributing Authors and Reviewers. LATMOS has been or still is involved in the following EU projects and networks: co-I for: FP5/POET, FP6/HYMN, FP7/ACCENT, FP7/Cityzen, FP7/MACC, FP7/PANDA.

It contributed to Eumetsat/O3M SAF for CDOP phase II and phase III since 2006, and participates to the ESA Climate Change Initiative (CCI-O3 project) since 2013.

1.1.1.6 Institute of Environmental Physics at the University of Bremen (IUP-UB)

The University of Bremen (UNI-HB or UB) is a medium size university with about 20,000 students. In 2012 it won the "Excellence Initiative" Award by the German government. The Institute of Environmental Physics (IUP), as part of the Physics/Electrical Engineering Department (Fachbereich 1) within the Universität Bremen, consists of three sections: "Physics and Chemistry of the Atmosphere" (Prof. J. P. Burrows), "Remote Sensing" (Prof. J. Notholt) and "Tracer Oceanography" (Prof. M. Rhein). IUP has approximately 110 employees, including students working for their masters and doctoral theses, scientific, and technical staff. The IUP team participating in C3S Ozone is part of the Section "Physics and Chemistry of the Atmosphere" led by Prof. John P. Burrows, SCIAMACHY PI and Lead Scientist of GOME.

The University of Bremen (UNI-HB) participates in two ESA CCI projects (ozone and GHG). In GHG_cci the IUP is project leader and in Ozone_cci leading the WP on limb ozone profiles. Main contribution to Ozone_cci is the ECV production of updated and improved SCIAMACHY limb ozone profiles and the harmonization of the available datasets of limb (high vertical resolution) ozone profiles with extended data records.

The Institute of Environmental Physics (IUP) of UNI-HB is one of the leading European research institutions in the field of ground- and space-borne remote sensing of the atmosphere. The satellite sensors GOME and SCIAMACHY were successfully proposed and supported by the IUP team since the early 1990's. IUP also proposed the CarbonSat mission, that was second in the final decision for the eighth ESA Earth Explorer mission.

The IUP team was directly involved in the SCIAMACHY definition and building phases and has been involved for more than 10 years in the development of innovative radiative transfer (e.g., SCIATRAN) and retrieval algorithms (e.g., DOAS, WFDOAS, BESD) for the analysis of GOME, SCIAMACHY, GOME-1, OMI, GOSAT, and Sentinel-5P data from the troposphere towards the mesosphere for gases such as O_3, NO_2, BrO, SO_2, H_2O, HCHO, CHOCHO, CH_4, CO_2 and CO as well as clouds (including NLCs and PSCs) and aerosol parameters.

IUP is involved in many different EU and ESA projects and has large experience in satellite remote sensing of atmospheric trace gases, from the scientific design of space instruments, retrieval techniques and data validation, to analyses of atmospheric data for applications in climate and ozone science.

1.1.1.7 Finnish Meteorological Institute (FMI)

The Finnish Meteorological Institute functions under the Ministry of Transport and Communications and has the mandate of producing weather, atmosphere, climate and marine related services

required by Finnish society. FMI provides reliable information on the state of the atmosphere, and its characteristics and phenomena, with the aim of promoting safety and serving various needs of the public, industry and commerce, as well as contributing to scientific ends. FMI makes observations of the physical state of the atmosphere, its chemical composition, and electromagnetic phenomena. FMI also develops and applies numerical models in order to analyse and forecast various atmospheric physical and chemical processes. FMI coordinates national satellite service centre in Sodankylä, which is also Copernicus Collaborative Ground segment. FMI employs about 680 people, about 350 of which are involved in research.

FMI's Earth Observation unit (FMI-EO) has expertise in middle atmosphere research including satellite instrument development, satellite remote sensing, middle atmosphere modelling, UV research, software applications. FMI-EO was an original co-proposer of the GOMOS stellar occultation instrument and has been closely involved through the entire period of mission definition, instrument definition, development, mission planning, operations planning, data processing algorithm development, development of in-flight calibration, geophysical validation and development of ground processing facilities. FMI is a member of the GOMOS Quality Working Group. FMI-Earth Observation is participating in a Swedish-led, Canadian, Finnish, and French small-satellite project Odin. FMI-EO has developed data retrieval algorithms and processors, currently used in the Sodankylä processing facility, for Odin's UV-visible spectrograph OSIRIS which uses limb scanning technique. FMI-EO is a co-PI of OMI (Ozone Monitoring Instrument) on-board the NASA mission EOS Aura and is leading the EUMETSAT's Ozone and Atmospheric chemistry Satellite Application Facility project.

The FMI Earth Observation Unit participates actively in the ongoing ESA Climate Change Initiative for ozone with responsibility of developing Level 3 data products from ozone profiles data by six satellite instruments. FMI has a practical experience in merging data from different platforms for creating long-term data record and in trend analyses. Other recent projects of FMI that are relevant for C3S ozone include ESA Climate Change Initiative for Aerosols, EUMETSAT O3M-SAF, EU GAIA-CLIM, ESA ALGOM, ESA MesosphEO.

1.1.2 System output

The C3S ozone data production system generates validated L3 and L4 ozone datasets (ozone total column, ozone tropospheric column, ozone profile) derived from satellite observations using nadir ultra-violet (UV) and thermal infrared (TIR) as well as limb and occultation techniques. Table 1 lists the products delivered by the system, with the basic characteristics of each of them. Additional characteristics of the ozone data products made available to C3S – and to the users via the C3S CDS – are detailed in the C3S Ozone Product User Guide and Specification (PUGS) [D8] while technical aspects of the production chains are described in the C3S Ozone Algorithm Theoretical Basis Document (ATBD) [D7].

Most of the C3S ozone data products have been developed as part of the ESA Ozone Climate Change Initiative project 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 the GCOS in the GCOS-107 report (WMO, 2006) (Product A.7: Profile and total column of ozone).

The C3S ozone data are freely available for download from the C3S Climate Data Store (CDS) at https://cds.climate.copernicus.eu/

Table 1. List of the C3S ozone data products available from the C3S CDS (March 2021). All products cover the globe and have a monthly temporal resolution. Data are provided in the NetCDF format.

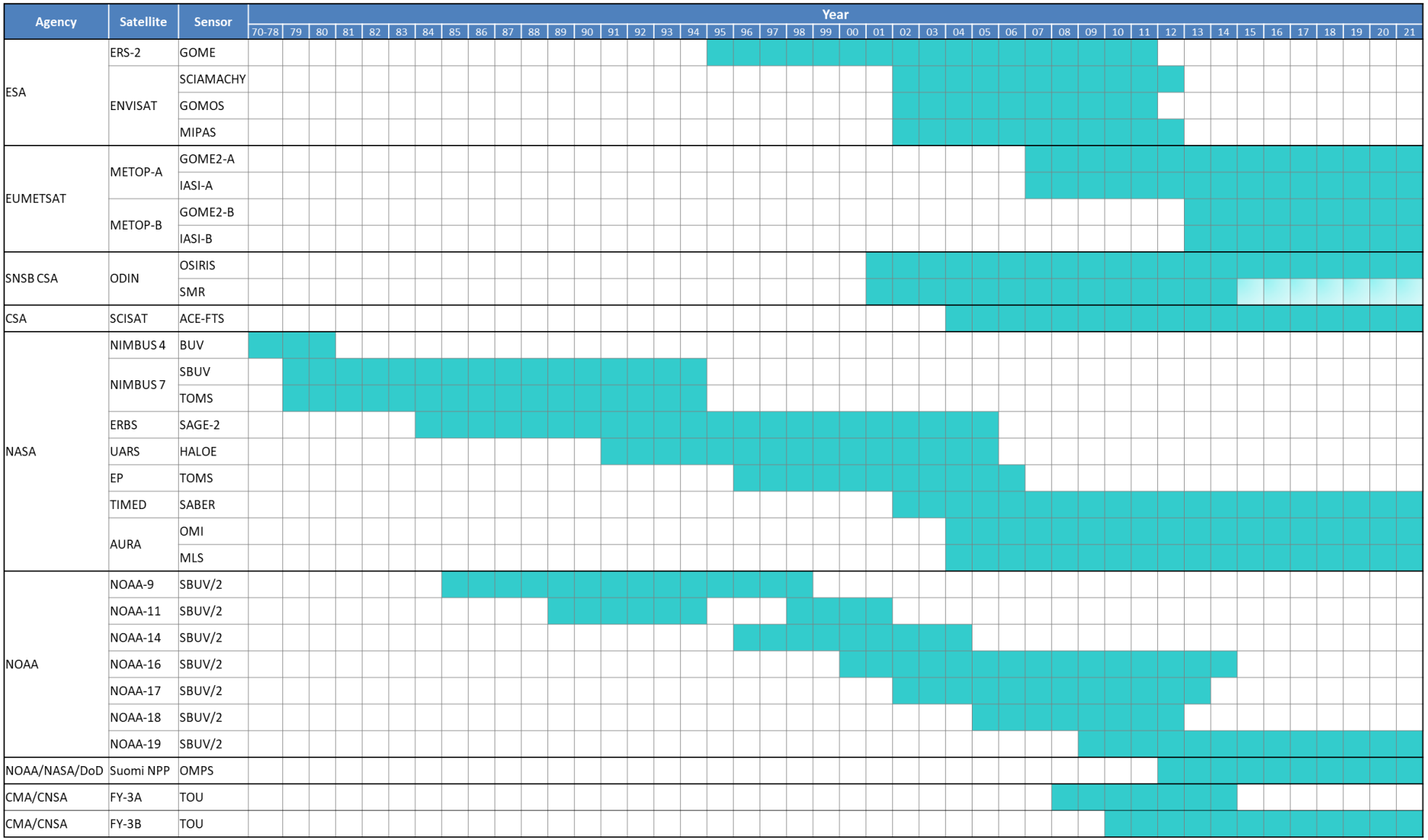
Product name	Product definition	Sensor(s)	Processing level	Product type	Overall temporal coverage	Update frequency	Spatial resolution	Uncertainty information	Provision & provenance
TC_GOME	Total ozone column	GOME	3	CDR	06.1995 - 07.2011	N/A	1°x1°	Random and smoothing error	BIRA/DLR
TC_SCIA		SCIAMACHY	3	CDR	08.2002 - 04.2012	N/A	1°x1°		BIRA/DLR
TC_GOME2A		GOME-2A	3	ICDR	01.2007 - 10.2020	Quarterly with 4 months delay	1°x1°		BIRA/DLR
TC_GOME2B		GOME-2B	3	ICDR	01.2013 - 10.2020		1°x1°		BIRA/DLR
TC_OMI		OMI	3	ICDR	10.2004 - 10.2020		1°x1°		BIRA/DLR
TC_OMPS		OMPS-NM	3	ICDR	01.2012 - 10.2020		1°x1°		BIRA/DLR
TC_GTO-ECV		GOME, SCIA, GOME-2A/B, OMI	3	ICDR	07.1995 - 10.2020	Semi-annually with 4 months delay	1°x1°	Random and sampling error	BIRA/DLR
TC_MSR		(1)	4	ICDR	04.1970 - 12.2020	Annually with 3 months delay	1°x1°	Forecast error cov.	KNMI
TC_IASI-A	Total and tropospheric ozone	IASI-A	3	ICDR	10.2007 - 01.2021	Quarterly with 1 month delay	1°x1°	Random error	LATMOS
TC_IASI-B		IASI-B	3	ICDR	05.2013 - 01.2021		1°x1°	Random error	LATMOS
06TC_IASI-A		IASI-A	3	ICDR	10.2007 - 01.2021		1°x1°	Random error	LATMOS
06TC_IASI-B		IASI-B	3	ICDR	05.2013 - 01.2021		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	ICDR	01.2007 - 10.2020	Annually with 4 months delay	1°x1°		RAL/KNMI
NP_GOME2B		GOME-2B	3	ICDR	04.2013 - 12.2017		1°x1°		RAL/KNMI
NP_OMI		OMI	3	ICDR	10.2004 - 10.2020		1°x1°		RAL/KNMI
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 - 12.2020	Annually with 3 months delay	10° lat zones		UNI-HB/FMI
LMZ_ACE		ACE	3	ICDR	02.2004 - 12.2020		10° lat zones		UNI-HB/FMI
LMZ_SABER		SABER	3	ICDR	01.2002 - 11.2020		10° lat zones		UNI-HB/FMI
LMZ_MLS		MLS	3	ICDR	08.2004 - 11.2020		10° lat zones		UNI-HB/FMI
LMZ_OMPS		OMPS-LP	3	ICDR	02.2012 - 12.2020		10° lat zones		UNI-HB/FMI
LMZ_MERGED		(2)	3	ICDR	10.1984 - 12.2020		10° lat zones		FMI
LP_MERGED		(3)	3	ICDR	11.2001 - 12.2020		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, BUV-Nimbus4, TOMS-Nimbus7, TOMS-EP, SBUV-7, -9, -11, -14, -16, -17, -18, -19, OMPS and TOU.
(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.

Figure 2 – Satellite sensors providing data used to derive C3S ozone data products.



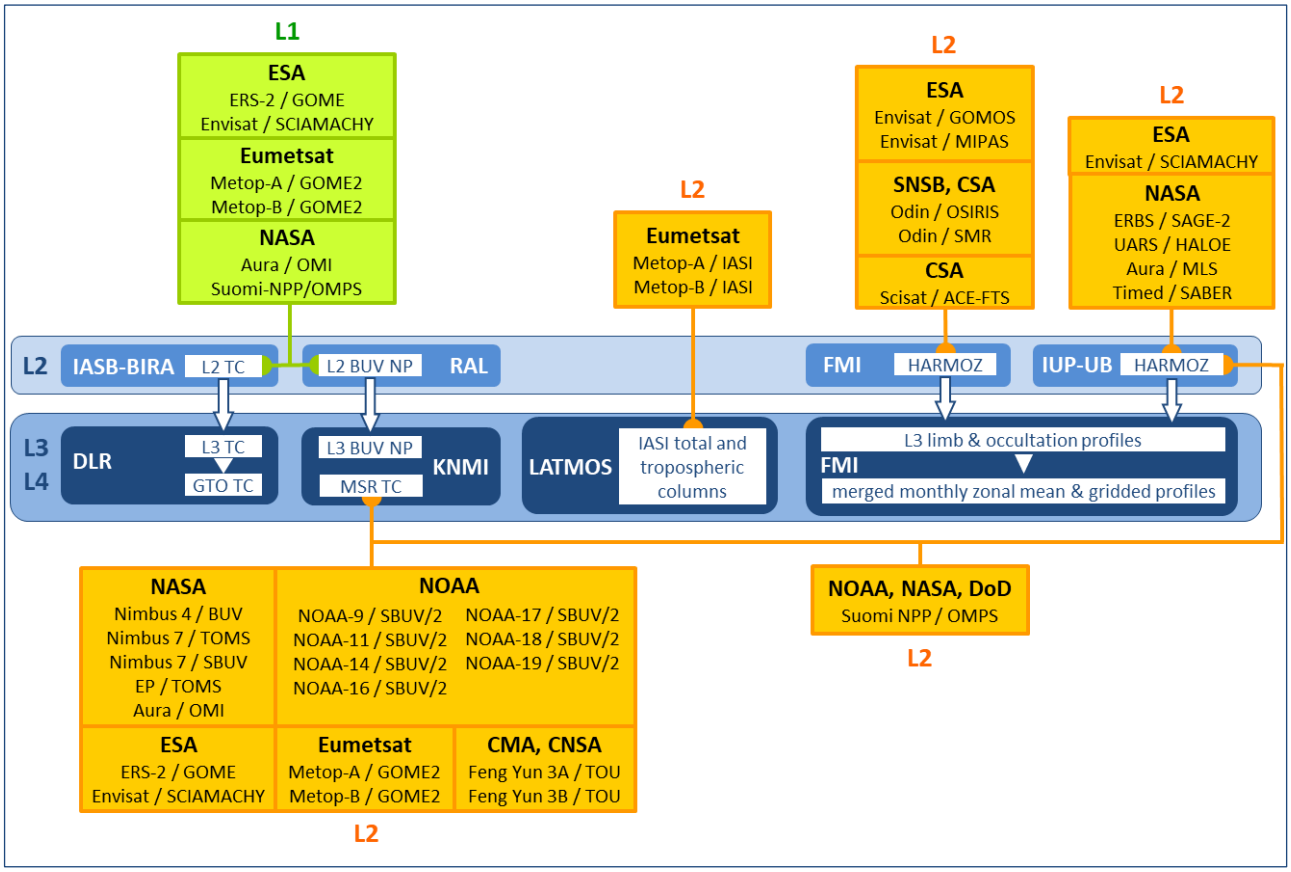
1.1.3 System input

1.1.3.1 Satellite data sources

The satellite sensors at the origin of the C3S ozone data are listed in **Fehler! Verweisquelle konnte nicht gefunden werden.**, which also shows, for each instrument, the operating agency and the observation time period covered.

Fehler! Verweisquelle konnte nicht gefunden werden. provides a schematic picture of which satellite data carrying information on the atmospheric ozone content are fed into the C3S ozone processing system to produce the different C3S ozone products (L3 and L4). These data are radiances (L1) for the retrieval of TOC and nadir profiles, ozone columns or profiles (L2) for the other products.

Figure 3 - L1 (in green) and L2 (in yellow) satellite data input to the C3S ozone processing system. The L2 products generated within the system (in light blue) are passed over to downstream parts of the system to generate the final L3 or L4 products (in dark blue) (see Section 1.1.4). TC = total column. NP = nadir profile.



Odin/SMR data were used under Contract C3S 312a Lot4 to produce the LMZ_SMR L3 ozone limb profile product. SMR is still in operation but the L1 data processing has been interrupted. It may resume later with the reprocessing of the entire data record.

Technical characteristics, provenance and providers of individual L1 and L2 input data are described in detail in the C3S Ozone ATBD [D7], Section 2.1 “Input data sets from satellites”.

1.1.3.2 Auxiliary data

Beside the L1 and L2 satellite data main input (carrying information on the ozone atmospheric content), the data processing requires a number of auxiliary datasets from various origins. Table 2 lists the auxiliary datasets used, with their provenance and application. Auxiliary data sets, including their originating systems, providers and associated delivery mechanisms, are described in detail in the C3S Ozone ATBD [D7], Section 2.2 "Ancillary data". Auxiliary data needed to retrieve L2 variables from L1 input are retained in Table 2 only when the retrieval is part of the tasks under the C3S contract. Accordingly, the atmospheric state data that serve as input to the FORLI retrieval scheme applied at LATMOS to IASI L1 data, although described in the ATBD, do not appear in Table 2. It is also true of auxiliary data required to derive L2 limb and occultation profiles from the L1 data (surface albedo gridded distribution, aerosol extinction profiles).

Table 2. Auxiliary variables required by the C3S ozone data processing system.

Physical quantity	Identification, provenance and provider	C3S application
Surface albedo spectral data	MLER climatological data derived from TOMS, GOME and OMI *(Herman and Celarier, 1997; Koelemeijer et al., 2003* and *Kleipool et al., 2008)* available from the TEMIS and OMI websites	Retrieval of ozone total column and nadir profile
Ozone profile global climatologies	➢ Combination of data from MLS and ozone sondes *(Labow et al., 2015)* available from TOMS website ➢ Tropospheric ozone climatology obtained by combination of OMI and MLS data *(Ziemke et al., 2011)* available from the NASA GSFC homepage for tropospheric ozone	Retrieval of ozone total column
Global digital elevation model (DEM)	GTOPO30 (on a 30 arc-sec horizontal grid) from USGS	Retrieval of ozone total column and nadir profile
Ozone UV absorption cross sections	➢ Brion, Daumont and Malicet (BDM) laboratory measurements *(Daumont et al., 1992 ; Malicet et al., 1995; Brion et al., 1998)* ➢ Laboratory data by *Gorshelev et al., 2014* and *Serdyuchenko et al., 2014* Both datasets are available from the authors and from public databases	Retrieval of ozone total column and nadir profile
Meteorological data (temperature, pressure)	IASI L2 meteorological data from Eumetsat	Creation of L3 total and tropospheric columns from IASI
Meteorological data (temperature, pressure)	ECMWF operational stratospheric analysis, ERA40, ERA-interim and ERA5	Retrieval of L2 nadir profiles, assimilation of total columns, harmonization of L2 limb profiles, creation of L3 profiles from L2 data

1.1.3.3 Reference validation data

Validation of the C3S ozone products is performed at IASB-BIRA (see Section 1.1.5) based on the independent reference datasets quoted in Table 3. Reference datasets and their providers are described in detail in the C3S Ozone Product Quality Assurance Document (PQAD) [D9], Section 3 "Description of validation datasets" and Appendix A "Details of validation data sets".

Table 3. Reference datasets used to validate the C3S ozone data products.

Reference dataset	Providers	C3S ozone products validated
Total ozone from Dobson and Brewer station network	WOUDC	Total ozone columns
Ozone partial pressure measured by balloon-borne ozone-sondes	NDACC, SHADOZ, WOUDC	➢ Tropical tropospheric column from IASI ➢ Nadir profiles from GOME, SCIAMACHY, GOME-2, OMI ➢ Zonal mean limb profiles from MIPAS, GOMOS, SCIAMACHY, SAGE-2, HALOE, OSIRIS, SMR, ACE, MLS, SABER ➢ Merged zonal mean limb profile ➢ Merged gridded limb profile

1.1.4 Distributed data processing system

A schematic representation of the distributed structure of the C3S ozone data processing system is provided in **Fehler! Verweisquelle konnte nicht gefunden werden.**, where arrows symbolize internal data flows. Data exchange takes place according to the teams' local exchange protocols. Details of the role of each component of the system are provided in the following sub-sections. Technical aspects of the production chains are described in the Algorithm Theoretical Basis Document (ATBD) [D7].

1.1.4.1 IASB-BIRA data processing system

This system generates L2 total columns (TC) of ozone from GOME, SCIAMACHY, GOME-2A, GOME-2B, OMI and OMPS L1 input data. The granularity is one orbit: there is one L2 product per orbit, per sensor. The system carries out the different steps necessary to the L2 TC production: ingestion of L1 and auxiliary data, processing of L1 data into L2 TC data, formatting of L2 product and uploading to the BIRA CDR database.

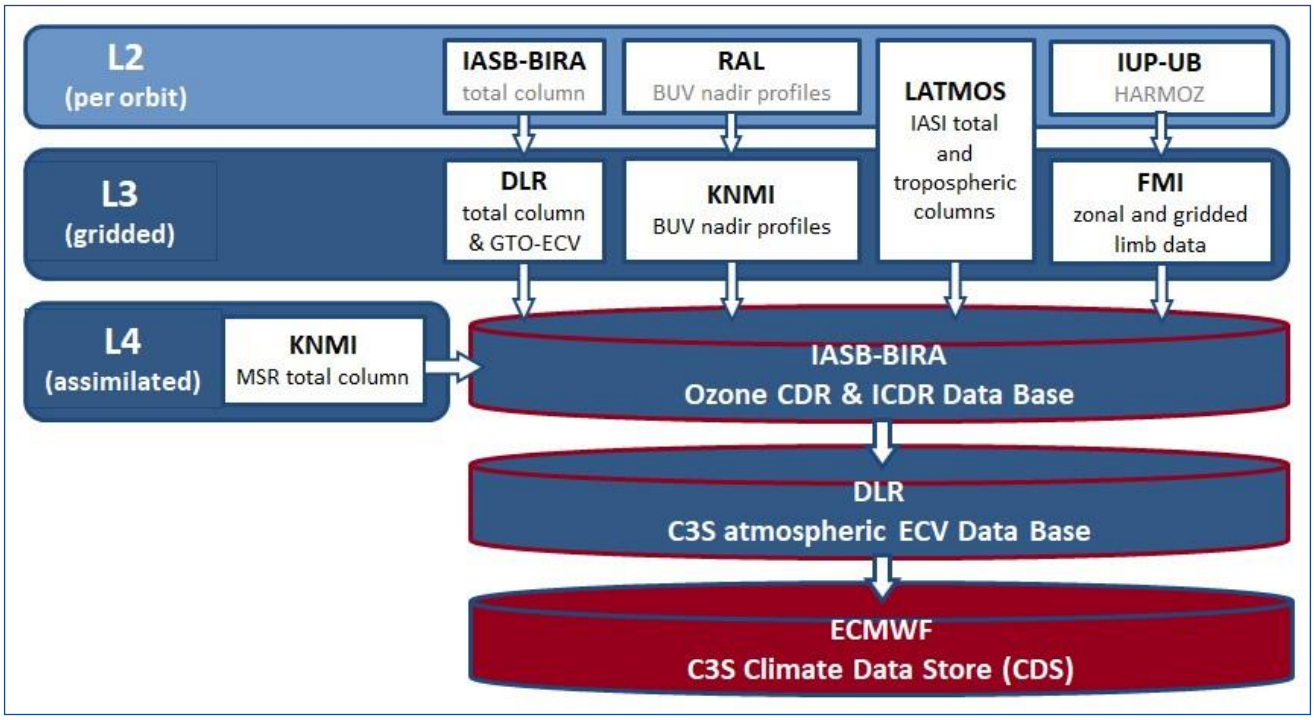
1.1.4.2 DLR data processing system

This processing system takes as input the L2 TC products from IASB-BIRA and generates the L3 TC products, i.e. gridded monthly mean total ozone data, separately for each sensor.

It also merges the L3 TC products by applying spatial and temporal drift corrections in order to create the final TC ECV from all available sensors (GTO-ECV).

The end products are uploaded to the IASB-BIRA CDR database.

Figure 4 – C3S ozone data distributed processing system.



1.1.4.3 RAL data processing system

This system generates L2 nadir profiles (NP) of the ozone concentration from the L1 data collected by the BUV sensors GOME, SCIAMACHY, GOME-2A, GOME-2B and OMI. The granularity is one orbit: there is one L2 product per orbit and per sensor. The system ensures the different steps necessary to the L2 NP production: ingestion of L1 and auxiliary data, processing of L1 data into L2 NP data, formatting of L2 product and uploading to KNMI and to the BIRA CDR database.

1.1.4.4 KNMI data processing system

This system uses the NP L2 products from RAL to generate NP L3 products, i.e. gridded ozone concentration profiles.

The system also produces L4 TC (TC_MSR) by assimilating L2 TC data from a series of GTO instruments, namely GOME, SCIAMACHY, OMI, GOME-2A/B, BUV-Nimbus4, TOMS-Nimbus7, TOMS-EP, SBUV-7, -9, -11, -14, -16, -17, -18, -19, TOU-FY3A/B and OMPS. The output of the assimilation is a single merged dataset combining the information provided by all the satellite instruments listed above.

The processing requires meteorological data to be provided by ECMWF.

The L3 and L4 datasets are uploaded to the IASB-BIRA CDR database.

1.1.4.5 LATMOS data processing system

This system generates the L3 NP products from the IASI L2 input data – also produced at LATMOS from the L1 input. The processing requires the availability of meteorological data. The IASI L2

meteorological data from the Eumetsat data centre are used. L2 and L3 datasets are uploaded to the BIRA CDR database.

1.1.4.6 IUP-UB data processing system

IUP-UB coordinates the harmonisation of the L2 limb and occultation profiles (HARMOZ). The IUP-UB system generates the harmonised L2 limb profile (LP) products including the UTLS information from the SCIAMACHY L2 input data. The harmonised L2 LP products for OMPS, MLS, SABER, SAGE II and HALOE are also generated within this system (Table 4). Harmonisation of additional L2 LP data is carried out at FMI (see Section 1.1.4.7 below).

Table 4. L2 datasets used to generate the harmonised L2 ozone products (HARMOZ) at IUP-UB.

Satellite	Sensor	L2 data provider
Envisat	SCIAMACHY	IUP-UB
ERBS	SAGE-2	NASA
UARS	HALOE	NASA
Aura	MLS	NASA
Timed	SABER	NASA
Suomi NPP	OMPS	IUP-UB

1.1.4.7 FMI data processing system

This system generates the harmonised L2 LP products from the GOMOS L2 input data including the UTLS and MLT information. It also generates the harmonised L2 LP products from MIPAS, OSIRIS, SMR and ACE-FTS (Table 5).

Table 5. L2 datasets used to generate the harmonised L2 ozone products (HARMOZ) at FMI.

Satellite	Sensor	L2 data provider
Envisat	GOMOS	ESA
	MIPAS	KIT
Odin	OSIRIS	ESA
	SMR	Chalmers
Scisat	ACE-FTS	ESA

Regarding the SMR data, see the note below the *List of datasets covered by this document* on Page 4.

On the basis of the harmonised L2 limb profiles produced at IUP-UB and FMI (HARMOZ), all L3 limb profile products from all individual sensors are generated at FMI.

Some of the resulting L3 LP products are merged to create two multi-instrument L3 datasets of ozone profiles:

LMZ_MERGED : Monthly zonal mean merged product based on MIPAS, GOMOS, SCIAMACHY, SAGE-2, OSIRIS, ACE and OMPS

LP_MERGED : Latitude-longitude gridded merged product based on MIPAS, GOMOS, SCIAMACHY and OSIRIS

1.1.5 Centralised data validation

Once uploaded to IASB (see Section 1.1.7), the C3S ozone products undergo a two-stage validation:

1. The first stage, which takes place before the data transfer to the DLR ECV data base, is a verification of the file metadata and file names (see Section 2.1).
2. Within three months following delivery to BIRA, the C3S ozone products listed in Table 3 (Column 3) are subject to the validation procedure documented in the C3S Ozone PQAD [D9]. File format and product coverage verifications are part of the validation process.

Details on the validated products, reference datasets and validation principles, methodology and results are provided in the C3S Ozone PQAD [D9] and PQAR [D4 and C3S_312b_Lot2 v1.1 delivery in May 2019].

Based on the estimators for bias, precision and stability computed by IASB-BIRA's validation system, the PQAD and PQAR also include an assessment of the compliance of the C3S ozone CDRs with target user requirements as published in the C3S Ozone Target Requirements and Gap Analysis Document (TRGAD) [D5] (Section 1.1.6).

These estimators are also used to quantify the key performance indicators (KPI) related to data quality, required by the project management.

1.1.6 User requirements and gap analysis

KNMI coordinates the compilation of user requirements related to atmospheric ozone data and the comparison of the C3S ozone product characteristics to the requirements, which leads to an in-depth analysis of the current gaps in the available products. This work is published in the C3S Ozone Target Requirements and Gap Analysis Document (TRGAD) [D5].

1.1.7 Data delivery

New L3 and L4 data versions and ICDR updates are uploaded to a restricted access area at BIRA-IASB where their providers are granted writing permission. After metadata and filenames are checked, files are moved to BIRA's C3S ozone CDR repository, which has read-only access from the outside world.

Delivery to the DLR ECV archive occurs according to a prescribed schedule (see Section 2). For the first C3S_312b_Lot2 delivery, the data have been transferred directly to the CDS, according to the procedure followed under C3S_312a_Lot4: ECMWF received the usual text file containing the list of all the paths to the corresponding products on BIRA's FTP server, which enabled the CDS to fetch the data and make them available to the public via the CDS web interface.

Within the following three months, the ozone data products are validated by BIRA-IASB as mentioned in Section 1.1.5 and data quality KPIs are re-evaluated (see Section 2).

1.2 Computing facilities

1.2.1 Royal Belgian Institute for Space Aeronomy (BIRA-IASB)

BIRA-IASB disposes of an important ICT infrastructure. The computing and storage capacity is fitted to perform total ozone level-2 processing. Facilities in place at BIRA include the following.

- Central file servers for scientific datasets (satellite & ground based measurement data):
  - 1.2 PB net capacity for datasets (06/2016).
  - Archiving to tape for older datasets.
  - All storage is configured for high availability.
  - The storage is configured in a cluster high performance data processing.
- Disaster recovery system for all data.
- Small Linux clusters for data processing and scientific modelling purposes (400+ x 86 compatible computing cores).
- Central high performance computing (HPC) server, shared with BIRA's Space-Pole partners RMI and ROB: HA Linux cluster with 2688 computing cores for HPC and operational tasks.
- Vmware Vsphere 5 based cluster for virtual servers. Fully redundant configuration.
- Web & Ftp servers for publishing and data exchange. Web servers are Linux/Apache-based with CMS or wiki application software.
- High-speed 10 Gbit/s Ethernet backbone, fully redundant 1 Gbit/s connection to the European research network & the internet.
- Eumetcast reception station for EUMETSAT/Metop data.
- ECMWF meteorological data available through special agreement.
- State-of-the-art compilers (Fortran 90/95, C/C++, etc.).
- Data Analysis tools (IDL, MatLab, etc.), and general purpose software.

1.2.2 German Aerospace Centre (DLR)

DLR is equipped with the resources and facilities that are necessary for the execution of the project. In particular, the following typical infrastructure resources are available:

- All team members are equipped with the most modern technology for "office facilities" (PCs, printers, MS Office, etc.).
- High quality network infrastructure, i.e. LAN at the individual DLR sites, WAN interconnecting the DLR sites and high speed internet access.
- Network security is implemented by central and de-central firewalls, desktop firewalls and virus protection.
- UNIX servers with Solaris and Linux operating systems as appropriate.
- Common IT services like central file service, backup service, license service, print service and mail service exist on a professional base.
- Communication services as telephone, email, web teleconferences using Adobe Connect.

1.2.3 Rutherford Appleton Laboratory (RAL)

RAL has access to the following facilities:

- JASMIN-CEMS computing facility, with 6000 cores (including 512 dedicated to the RAL group) and 30 Petabytes of storage (see http://www.jasmin.ac.uk/) in addition to the group's dedicated cluster of Linux computers comprising ~200 cores.
- Satellite L1 data sets and auxiliary met analysis / re-analysis data from ECMWF required for production of ozone data are resident on JASMIN-CEMS.
- A range of radiative transfer codes including fast approximate models (e.g. RTTOV and the LUT based model used in ORAC) and reference scattering codes for modelling scattering in 1-D and 3-D (e.g. DISORT, SHDOM).
- State-of-the-art atmospheric optical property data-sets and models.
- Full range of analysis software, including IDL.
- Standard tools for software development support (C, FORTRAN compilers, configuration control tools SVN, RCS, CVS etc.)

1.2.4 Royal Netherlands Meteorological Institute (KNMI)

The facilities of KNMI comprise reception of satellite data via satellite link, ftp-servers, the information and data management facility including the archive and the user services providing access to products and services. In more detail the elements being used are the following.

- As PI institute of OMI KNMI has access to all OMI data in the Data Archive Centre of NASA.
- As national SCIAMACHY data centre KNMI has a large data storage facility including a complete archive of the official SCIAMACHY data products.
- As national meteorological organisation KNMI has access to the meteorological data of ECMWF.
- As national institute for distribution of measurements from the EUMETSAT meteorological satellites KNMI has access to Meteosat and MSG data. KNMI has an operational receiving station for MSG data since May 2003.
- KNMI has dedicated high performance computing facilities

1.2.5 Laboratoire Atmosphères et Observations Spatiales (LATMOS)

The C3S ozone activities are performed in the LATMOS laboratory at University Pierre-et-Marie-Curie inside Paris. The facility is equipped with fast data connection and large computing power and storage capacity, including a multi CPU cluster (CICLAD) to process the IASI data. This cluster is maintained by IPSL (Institut Pierre Simon Laplace) at UPMC and is shared with the other laboratories part of IPSL.

It includes 7 nodes :

- 4 computers 64 processors (RAM 256Go)
- 1 computer 32 processors (RAM 128 Go)
- 2 computers 8 processors (RAM 32 Go)

The project benefits from LATMOS computer staff for technical support and assistance.

1.2.6 Institute of Environmental Physics at the University of Bremen (IUP-UB)

The IUP has a large computational capacity, which is essential for extensive retrieval studies and for the processing and analysis of large data sets from satellite sensors. It has access to a variety of workstations and servers:

- local Linux cluster of twelve two-dual-quadcores (thus 8 cores/nodes) based on Intel processors E5345 running with 2.3 GHz, ten two-hexacores (thus 12 cores/node) based on Intel processors X5675 running with 3.07GHz, and three sixteen cores based on intel processors E5-2637v2 with 3.5 Ghz, totalling 264 cores;
- IUP dedicated HPC in the Physics Department with 12 blades each consisting of two quadcore X5570 Intel processors (2.9 GHz);
- Shared memory system based on IBM power7 processors with 64 cores running typically 256 threads;
- HPC for parallel applications with 28 nodes, each consisting of two octacores (32 thread) with E-2667v3 Intel processors running with 3.2 GHz;
- several storage raids totalling about 1.1 Pb, holding among others SCIAMACHY, MERIS, GOME, and GOME-2 level-1 and level-2 data.

IUP also has a significant contingent from a high performance computer within the Physics Department, the latter is associated with the North-German Supercomputing Alliance (Norddeutscher Verbund zur Förderung des Hoch- und Höchstleistungsrechnens - HLRN) in Hannover, Germany.

1.2.7 Finnish Meteorological Institute (FMI)

The C3S ozone activities are performed at the FMI-EO and FMI premises at Helsinki and Sodankylä, respectively. These facilities are equipped with fast data connection. The ozone data from GOMOS/Envisat are readily available at FMI-EO. There is a full suite of atmospheric measurements at Sodankylä related to ozone research, including ozone sondes, hygrometer sondes, radiosondes, campaign-based aerosol sondes, spectrometers, MW radiometers, FTIR.

The Finnish Meteorological Institute has modern computing facilities and networks to serve its diverse tasks in both operational weather services and a wide range of research activities. The FMI computing system consists of two identical Cray XC-30 with 3320 processors each, online total disk space of ~0.5 PB and expandable tape-based long-term storage. To ensure its mandate as national weather service, FMI has established an institute-wide data security policy to ensure data integrity, data confidentiality and data availability in all situations.

In everyday use the project personnel uses modern office software (MS Office, OpenOffice), operating systems (Windows, Os X, Ubuntu Linux) and special-purpose software for different tasks, such as Matlab for mathematical analysis, MS Project for project management and a wide range of programming languages and environments (FORTRAN, C, C++, Java, Python, etc).

2. Upgrade cycle implementation procedure

2.1 General procedures

2.1.1 Data and key performance indicators (KPI)

Under C3S 312b Lot2, only one version of the historical ozone CDR was scheduled, at the end of the contract (28/02/2021). ICDR are completed at regular time intervals with newly processed data (quarterly, semi-annually or annually depending on the ICDR – see the *List of datasets covered by this document* on Page 4 and **Table 1** on Page 24, Column 7, *Update frequency*). The data quality KPIs are re-evaluated at the time of every delivery.

The upgrade cycle procedure is implemented as follows.

- As delivery time comes close, BIRA sends a reminder to its partners, who upload data updates to BIRA's FTP server as described in Section 1.1.7.
- File metadata and file names are checked.
- Data files are transferred to IASB-BIRA's dedicated C3S ozone data repository.
- DLR is informed of the new data availability and of all the paths to the corresponding products in the repository.
- DLR downloads the new data.
- Data validation is performed within the following three months (see Section 1.1.5) and data quality KPIs are re-evaluated.
- KPI values are reported in the C3S 312b Lot2 quarterly reports.

2.1.2 Documentation

An overview of the C3S ozone data products is provided on the C3S Climate Data Centre (CDS) at https://cds.climate.copernicus.eu/cdsapp#!/dataset/satellite-ozone-v1?tab=overview
The top of that webpage is shown in **Figure 5**.

Essential documents accompany the data produced under C3S 312b Lot2. Their titles are self-explanatory. The documents are collected and compiled by DLR for all C3S 312b Lot2 ECVs. Several issues are scheduled for each of them. Table 6 provides the list of the issues related to the ozone products. If no change has occurred since the previous issue, the new issue will reproduce the previous one. If necessary, the documents may undergo updates at a higher frequency.

The last issue of each document is made available to the users on the C3S Climate Data Centre (CDS) website under the thumbnail "Documentation" (see **Figure 5**).

Figure 5 – C3S ozone dataset home page of the CDS website.

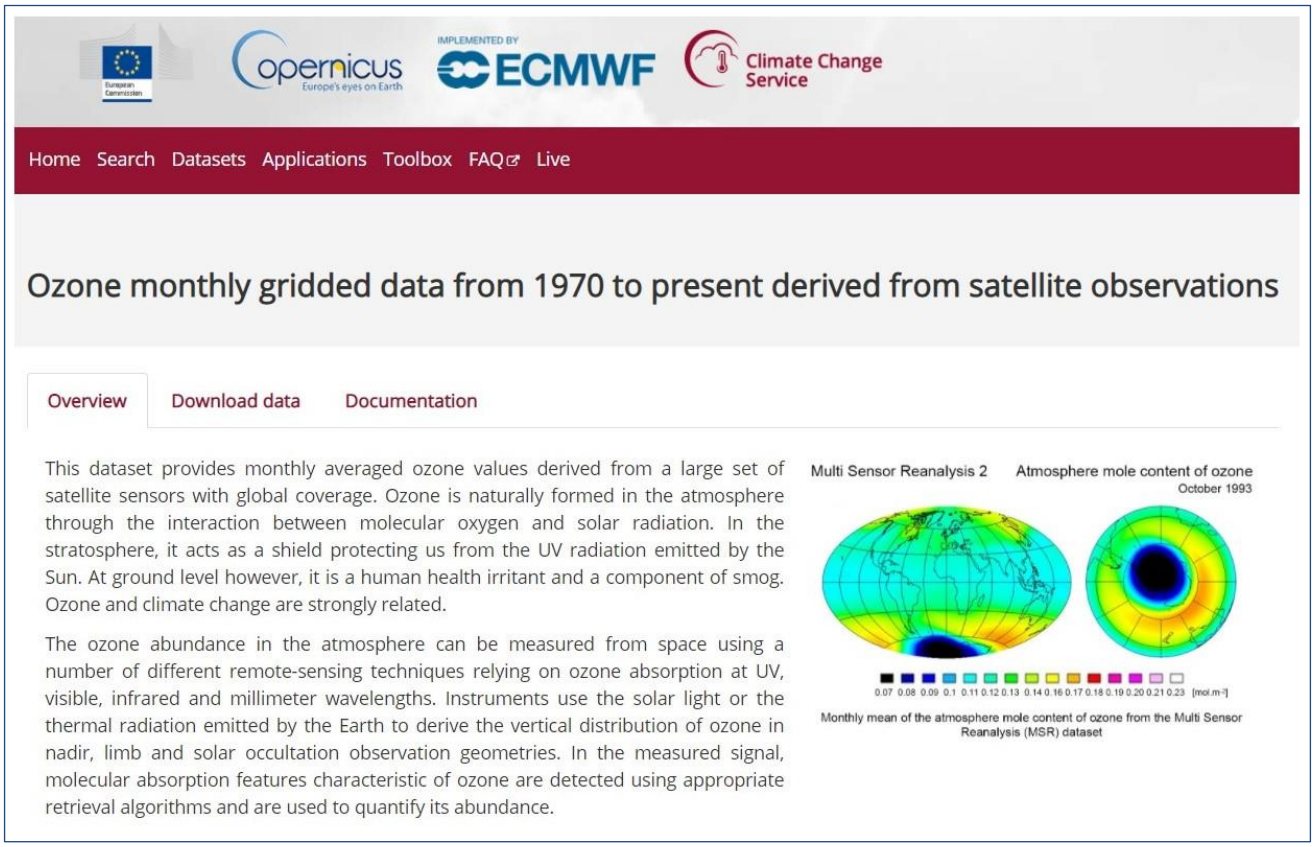


Table 6. Documents accompanying the C3S ozone data.

Document title	Acronym	Version	Due delivery date
Algorithm Theoretical Basis Document	ATBD	1.1	28.2.2019
		2.0 [D7]	28.2.2021
Product Quality Assurance Document	PQAD	1.1	28.2.2019
		1.2	28.2.2020
		2.0 [D9]	28.2.2021
Product User Guide and Specification	PUGS	1.1	28.2.2019
		1.2	28.2.2020
		2.0 [D8]	28.2.2021
Product Quality Assessment Report	PQAR	1.1	31.5.2019
		1.2	31.5.2020
		2.0	31.5.2021
Gap Analysis and Target Requirements Document	TRGAD	2018	31.12.2018
		2019	31.12.2019
		2020 [D5]	31.12.2020
System Quality Assurance Document	SQAD	1	31.3.2019
		2	30.9.2019
		3	31.3.2020
		4	30.9.2020
		5 [this document]	31.3.2021

Document title	Acronym	Version	Due delivery date
Annual Implementation Report	AIR	2018	28.2.2019
		2019	28.2.2020
		2020	28.2.2021
		final	31.8.2021

In addition to the key information recorded in the above documents, progress made in terms of data processing and all other related tasks are reported in the C3S Ozone quarterly reports, which also include the updated table of KPIs.

2.2 Specific procedures

2.2.1 Ozone total column from nadir sensors

2.2.1.1 Level 2

L2 total ozone data sets are updated every 3 months. This update requires first to update the OMI data time series, which is then used as the reference to compute L1 soft-calibration factors computed for the GOME-2 instruments aboard the platforms Metop-A and –B and for the OMPS instrument. Based on these updated soft-calibration factors, the GOME-2A/B and OMPS time series are then extended. Newly reprocessed data are then uploaded on the ozone_cci ftp server and made available to the L3 team for the TC ECV production.

2.2.1.2 Level 3

For the total ozone L3 CDRs TC_GOME and TC_SCIA upgrades are performed only in the wake of reprocessings of the data records (see Section 3.1.2).

For the total ozone L3 ICDRs TC_GOME2A, TC_GOME2B, TC_OMI and TC_OMPS, upgrades are performed quarterly with 4 months delay. The ICDRs are then extended and completed with the newly processed data and finally delivered to the BIRA FTP server.

The merged total ozone level 3 ICDR TC_GTO-ECV is upgraded semi-annually with 4 months delay. Newly processed data from the individual sensors are integrated in GTO-ECV and the ICDR is extended by 3 months. Owing to the merging approach that is applied [D7], every upgrade affects the TC_GTO-ECV (in terms of minor changes in total ozone columns) from 2007 (beginning of GOME-2A period) to the end.

2.2.2 Multi-sensor total ozone reanalysis (MSR)

Annually all satellite data and WOUDC ground observations are collected. Corrections are derived using the WOUDC data base and applied to all satellite data sets. After this the corrected satellite data is assimilated with TM4DAM using the ERA-interim meteorological data. Preparations to assimilate the entire time period using ERA5 are ongoing.

2.2.3 Ozone total and tropospheric columns from IASI

Each new data cycle is implemented quarterly. A first step consists of gridding the data (each month), a second step consists in generating the netcdf files (quarterly).

2.2.4 Ozone profiles from nadir sensors

2.2.4.1 Level 2

L2 ozone nadir profile data sets are updated yearly. For the GOME-2 instruments, this update requires an update to the L1 radiometric soft-calibration factor (based on a mission to date comparison with climatology). This correction has been held constant since 1st Jan 2017 to avoid discontinuities in the time-series. For GOME-2B, L1 radiometric issues have prevented sufficient quality nadir profile data being processed beyond December 2017 (to be addressed in the Ozone cci). For OMI, no soft calibration is required. Newly processed data are then made available to the L3 team for the ECV production.

2.2.4.2 Level 3

The level 2 ozone profiles from Section 2.2.4.1 are processed to level 3 files in the same cycle.

2.2.5 Ozone profiles from limb and occultation sensors

2.2.5.1 HARMOZ

The system generates level 2 ozone profiles from MLS, SABER, and OMPS, which are harmonized using ECWMF ERA5 data. The harmonized L2 limb profile (LP) dataset is then transferred to FMI to produce the L3 limb profile products.

2.2.5.2 Level 3

All processed datasets are checked by the data creator (both technical and information aspects). For the merged datasets, an additional checking as a long-term dataset is performed.

3. Procedures for reprocessing CDRs

Reprocessing of ozone CDRs happens only when significant changes to the processing algorithms or to the input data take place. It is therefore determined by the R&D activities conducted outside of C3S (ESA Ozone_cci+ project), and obeys their schedule.

3.1 Ozone total column from nadir sensors

3.1.1 Level 2

It is foreseen that L2 total ozone data sets are reprocessed only in case of significant retrieval algorithm update or in case of major change in the input data affecting significantly the products. In case of reprocessing, the procedure would be similar to the procedure followed to update the time series (see Section 2.2.1.1).

3.1.2 Level 3

For the total ozone L3 CDRs TC_GOME and TC_SCIA, and the ICDRs TC_GOME2A, TC_GOME2B, TC_OMI, TC_OMPS and TC_GTO-ECV, complete reprocessings are performed only after reprocessings of the corresponding level 2 data sets (see Section 3.1.1). For the combined total ozone TC_GTO-ECV data record, reprocessing occurs if significant changes are made to the merging algorithm applied to generate the CDR.

3.2 Multi-sensor total ozone reanalysis (MSR)

Reprocessing takes place when new level 2 data sets have been generated for previous years.

3.3 Ozone total and tropospheric columns from IASI

The complete IASI Level-3 dataset is likely to be reprocessed in case of any major changes in the IASI Level-2 O_3 products, which can be related to either a change in the FORLI-O3 version (mainly because of major updates within the code) or the generation of new quality flags.

3.4 Ozone profiles from nadir sensors

3.4.1 Level 2

It is foreseen that L2 ozone nadir profile data sets are reprocessed only in case of significant retrieval algorithm update or in case of major change in the input data affecting significantly the products. In case of reprocessing, the procedure would be similar to the procedure followed to update the time series (see Section 2.2.4.1).

3.4.2 Level 3

Reprocessing takes place only when the level 2 (see Section 3.4.1) has been reprocessed.

3.5 Ozone profiles from limb and occultation sensors

The main effort is creating the Level 2 data. Additional analyses for data assessment are needed. They include analyses of biases and drift. Also updates in filtering of invalid data are needed.

If an updated dataset will have a different (larger) altitude range, external parameters (atmospheric temperature and air density) from meteorological models will require updates.

Production of Level 3 data from HARMOZ files is straightforward and requires usual procedure for data production and quality control.

Depending on updated dataset, the production of merged datasets might require full reprocessing. Since the creating of the merged datasets is rather fast, this is expected to be feasible.

4. System maintenance and system failures

Each part of the data processing system applies specific procedures to maintain the system and deal with failures.

4.1 Ozone total column from nadir sensors

4.1.1 Level 2

Four level-2 data sets co-exist, which allows for a quality monitoring of each of them. In addition, correction factors generated as part of the L3 production also serve as an indicator of the data quality. The BIRA-IASB storage server possesses backup capability, providing recovery possibility in case of system failure. In case of interruption of the L1 flow for any of the instruments currently in operation, the other three are expected to continue to operate ensuring a continuous provision of the L3 record.

4.1.2 Level 3

The processing system to generate the level 3 (I)CDRs from the individual nadir sensors and the merged TC_GTO-ECV ICDR contains basic procedures to deal with possible failures, i.e. elementary quality checks are routinely applied to the output data.

4.2 Multi-sensor total ozone reanalysis (MSR)

The MSR depends on meteorological data, which is currently ERA_interim. Preparations to assimilate the entire time period using ERA5 are currently ongoing.

4.3 Ozone total and tropospheric columns from IASI

LATMOS and ULB have their own antenna to get IASI L1C and L2 data. In case of temporary data transfer interruption at LATMOS, the data are recovered in near real time at ULB (and vice versa).

In case of any instrument failure (for example IASI-A), the IASI-B data can be used instead (and vice versa).

4.4 Ozone profiles from nadir sensors

4.4.1 Level 2

The RAL processing is performed on the UK JASMIN computer infrastructure, which is also located at RAL and well supported. A copy of the GOME-2A & B L1 data is routinely acquired by and stored on the UK CEDA datastore, also housed on the JASMIN infrastructure. The Group also hold a copy of the GOME, SCIAMACHY and OMI L1 data on JASMIN. The OMI data is downloaded from NASA as required. Computer infrastructure maintenance is performed to minimize downtime to the community. In the event of significant disruption, DLR and ECMWF will be notified of any potential impacts as early as possible.

4.4.2 Level 3

No problems foreseen. The software can run on various systems.

4.5 Ozone profiles from limb and occultation sensors

IUP-B downloads the MLS and SABER data via internet on a monthly basis. Also, the ECWMF ERA5 data are constantly updated. The ECWMF data has a lag of 2 months with respect to the profile data.

5. User support

Support is provided to the users of C3S ozone data in different ways.

5.1 Fundamental supporting documents

Essential documents are produced and made available to the users via the C3S CDS interface (see Section 2.1.2).

The primary source of information on C3S ozone products is the Product User Guide and Specification (PUGS) [D8], which provides a description of each type of ozone products (L3 or L4, columns or profiles, nadir or limb technique), including originating sensor, temporal coverage, some information on the retrieval algorithm, bias corrections performed, target requirements, file format and names, quality indicators and other information supporting data usage. Product technical specifications are provided in the four annexes to this document.

The Algorithm Theoretical Basis Document (ATBD) [D7] 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 Product Quality Assurance Document (PQAD) [D9] describes the validation method applied to the data while the Product Quality Assessment Report (PQAR) [D4] gives an account of the validation results and provides an assessment of the data compliance with user requirements exposed in the Target Requirements and Gap Analysis Document (TRGAD) [D5].

5.2 Frequently asked questions (FAQ)

The front-end user support is provided by the CDS User Support (CUS) team based on an initial list of fifteen expected frequently asked questions (FAQ) and their answers, that have been provided to ECMWF by the product developers' teams under Contract C3S_312a_Lot4 [D3]. The list of these FAQ and their answers is provided in Table 7.

Table 7. C3S ozone frequently asked questions (FAQ) and answers.

Ozone data products
1. Which data processing levels are provided here for ozone? Level 3 and Level 4.
2. How can I retrieve a particular dataset? By selecting the right entries on the Copernicus CDS webpage for ozone at https://cds.climate.copernicus.eu/cdsapp#!/dataset/satellite-ozone-v1?tab=form
3. What are the main differences between L2 and L3 Ozone products?

The variables in L3 files are mapped on a uniform space-time grid, whereas the L2 variables are geo-located at the space-time position of the original measurements.

4. Where can I find a general overview of all ozone products and a description of the ozone variables they include?

   An overview of the C3S ozone datasets is provided in the C3S Ozone home page ***Ozone monthly gridded data from 1970 to present derived from satellite observations*** of the CDS website (see **Figure 5**, Page 36), at

   https://cds.climate.copernicus.eu/cdsapp#!/dataset/satellite-ozone-v1?tab=overview

   The C3S Ozone Product User Guide and Specification document (PUGS) [D8] provides a detailed description of each data product. The most recent version of the PUGS and of all the other documents pertaining to C3S ozone datasets can be accessed from that page by clicking on the *Documentation* thumbnail, or *via* the URL link

   https://cds.climate.copernicus.eu/cdsapp#!/dataset/satellite-ozone-v1?tab=doc

5. What is the difference between CDR and ICDR product types?

   For a CDR (Climate Data Record) the temporal coverage is fixed. An ICDR (Intermediate Climate Data Record) is extended in time at regular intervals and can therefore only be generated from active sensors. For more details concerning the extension in time, please consult the Product User Guide and Specification document (PUGS) [D8].

   In the CDS, only the most recently updated version of ICDRs is mentioned as being an ICDR, previous versions being considered as completed CDRs.

6. Is the information on the algorithms used for data processing available for users to access?

   A detailed algorithm description is provided for each data product in the ATBD (Algorithm Theoretical Basis Document) [D7]. The most recent version of the ATBD is available from the C3S ozone documentation page at

   https://cds.climate.copernicus.eu/cdsapp#!/dataset/satellite-ozone-v1?tab=doc

7. I have a specific question about a data product, can I contact the science team directly?

   No, please raise your question to the Copernicus C3S Helpdesk User Support Service through their web-form at https://cds.climate.copernicus.eu/contact-us

   If needed, your question will be forwarded to the appropriate science team(s).

Data processing and quality assurance

8. Is the information pertaining to quality assurance for the data products available for users to access?

Yes, this information is provided in the PQAD (Product Quality Assurance Document) [D9], the last version of which is available on the CDS ozone webpage at

https://cds.climate.copernicus.eu/cdsapp#!/dataset/satellite-ozone-v1?tab=doc

Data access

9. Where can I access ozone products/data?

   At https://cds.climate.copernicus.eu/cdsapp#!/dataset/satellite-ozone-v1?tab=form

10. What other products/data is available on the CDS?

    The C3S Climate Data Store provides data and information on Essential Climate Variables (ECV). The searchable catalogue of all the available datasets can be found at

    https://cds.climate.copernicus.eu/cdsapp#!/search?type=dataset

11. Do I have to register/pay for data access?

    Data can be used for free under the terms and conditions of the *License to use Copernicus products* provided on the download page at

    https://cds.climate.copernicus.eu/cdsapp#!/dataset/satellite-ozone-v1?tab=form

    Registering is however necessary (click on the *Login/register* box in the top right corner of the page).

12. Are there terms and conditions to using these products/data?

    Yes. They are available at

    https://cds.climate.copernicus.eu/cdsapp#!/dataset/satellite-ozone-v1?tab=form

    (click on *License to use Copernicus products* on the right hand side of the page).

Data format and tools

13. What formats are the ozone products provided in?

    All ozone CDR files are provided in netCDF4-CF format. Many programming languages provide open-source libraries for I/O of these binary files. These files can be opened with a viewer such as HDFView (free of charge, but requires a Java environment). The CDS toolbox provides routines to handle the files.

Other esources

14. What other resources of information are available for the ozone data/products?

Fundamental documents accompanying the data can be downloaded from the CDS website under the *Documentation* thumbnail:

- C3S ozone algorithm theoretical basis document (ATBD)
- C3S ozone product user guide and specification (PUGS)
- C3S ozone product quality assurance document (PQAD)
- C3S ozone product quality assessment report (PQAR)
- C3S ozone target requirements and gap analysis document (TRGAD)

The CDS toolbox allows users to write Python scripts to download data files, retrieve data subsets and to handle, process and plot data. Examples of simple applications are provided.

User support

15. Where can I get additional support on using the ozone data?

If you can't find the answer to your query in this FAQ, or in any of the other documentation provided, then we advise that you contact the Copernicus User Support (CUS) team at https://cds.climate.copernicus.eu/contact-us

5.3 Help desk

All questions and comments related to Copernicus data products

(including the ones described in this document)

shall be submitted via this website:

https://cds.climate.copernicus.eu/contact-us

References

Bojinski, S., M. Verstraete, T. C. Peterson, C. Richter, A. Simmons and M. Zemp, The concept of essential climate variables in support of climate research, applications and policy, Bulletin of the American Meteorological Society (BAMS), 1431-1443, September 2014. http://www.wmo.int/pages/prog/gcos/documents/bams_ECV_article.pdf

Fussen, D., and C. Bingen, A volcanism dependent model for the extinction profile of stratospheric aerosols in the UV-visible range, *Geophys. Res. Lett.,* 22, 703-706, 1999.

Herman, J.R. and E. A. Celarier, Earth surface reflectivity climatology at 340-380 nm from TOMS data, J. Geophys. Res., 102, 28003-28011, 1997.

Kleipool, Q.L., M.R. Dobber, J.F. De Haan and P.F. Levelt, Earth Surface Reflectance Climatology from Three Years of OMI Data, J. Geophys. Res, 113, D18308, doi:10.1029/2008JD010290, 2008.

Koelemeijer, R. B. A., J. F. de Haan and P. Stammes, A database of spectral surface reflectivity in the range 335–772 nm derived from 5.5 years of GOME observations, J. Geophys. Res., 108, NO. D2, 4070, doi:10.1029/2002JD002429, 2003.

Labow, G. J., Ziemke, J. R., McPeters, R. D., Haffner, D. P. and Bhartia, P. K.: A Total Ozone Dependent Ozone Profile Climatology based on Ozone-Sondes and Aura MLS Data, J. Geophys. Res. Atmos., n/a-n/a, doi:10.1002/2014JD022634, 2015.

Matthews, E., Global vegetation and land use: new high resolution data bases for climate studies, *J. Clim. Appl. Meteo.,* 22, 474-487, 1983.

National Research Council, Climate Data Records from Environmental Satellites: Interim Report 2004, 150 pp., ISBN: 978-0-309-09168-8, DOI: https://doi.org/10.17226/10944, 2004.

Parkinson, C., A. Ward and M. King, Earth Science Reference Handbook, NASA, Washington DC, 2006.

Werschek, M., EUMETSAT Satellite Application Facility on Climate Monitoring, C3S Climate Data Store workshop, Reading, UK, 3-6 March 2015. http://www.ecmwf.int/sites/default/files/elibrary/2015/13546-existing-solutions-eumetsat-satellite-application-facility-climate-monitoring.pdf

WMO, Systematic Observation Requirements for Satellite-based Products for Climate: Supplemental details to the satellite-based component of the Implementation Plan for the Global Observing System for Climate in Support of the UNFCCC, GCOS-107, 2006. https://library.wmo.int/doc_num.php?explnum_id=3813

Ziemke, J. R., Chandra, S., Labow, G. J., Bhartia, P. K., Froidevaux, L., and Witte, J. C.: A global climatology of tropospheric and stratospheric ozone derived from Aura OMI and MLS measurements, Atmos. Chem. Phys., 11, 9237-9251, doi:10.5194/acp-11-9237-2011, 2011.

Copernicus Climate Change Service

ECMWF - Shinfield Park, Reading RG2 9AX, UK

Contact: info@copernicus-climate.eu

climate.copernicus.eu copernicus.eu ecmwf.int