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Target Requirements and Gap Analysis Document

Ozone ECV

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2.0	06.03.2020	Cross-harmonisation within Lot2	Whole document
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5.3	03.01.2024	December 2023 update	Whole document

5.4	16.02.2024	Formatting corrections	Whole document

Related documents

Reference ID	Document
D1	GCOS, 2016, The Global Observing System for Climate: Implementation Needs. GCOS-200, WMO, Geneva, October 2016, https://unfccc.int/sites/default/files/gcos_ip_10oct2016.pdf
D2	van Weele, M. and the Ozone_cci science team, 2021, Ozone_cci+ User Requirement Document (URD), Version 3.1, Ozone_cci_URD_3.1, 5 March 2021, https://climate.esa.int/media/documents/Ozone_cci_urd_v3.1_version_05032021.pdf
D3	van Weele, M., Müller, R., Riese, M., Engelen, R., Parrington, M., Peuch, V.-H., Weber, M., Rozanov, A., Kerridge, B., Waterfall, A., and Reburn, J., 2015, User requirements for monitoring the evolution of stratospheric ozone at high vertical resolution, 'Operoz', Operational ozone observations using limb geometry. ESA report, Expro Contract: 4000112948/14/NL/JK, https://books.google.be/books/about/User_Requirements_for_Monitoring_the_Evo.html?id=Bv5QzgEACAAJ&redir_esc=y
D4	E.U. Copernicus Climate Change Service (2018), C3S_312a_Lot4 Ozone Target Requirement and Gap Analysis Document, TRGAD_v1, C3S_312a_Lot4.1.1.1_201803_TR_GA_v1
D5	E.U. Copernicus Climate Change Service (2020), C3S_D312b_Lot2 Ozone Target Requirements and Gap Analysis Document, TRD-GAD v3.0, C3S_D312b_Lot2.1.0-2020(O3)_TRD-GAD_v3.0
D6	The 2022 GCOS Implementation Plan, GCOS-244, WMO, Geneva, 2022, https://library.wmo.int/doc_num.php?explnum_id=11317
D7	The 2022 GCOS ECVs Requirements, GCOS-245, WMO, Geneva, 2022, https://library.wmo.int/doc_num.php?explnum_id=11318
D8	E.U. Copernicus Climate Change Service (2021), C3S_D312b_Lot2 Product Quality Assessment Document, PQAD v2.0, C3S_D312b_Lot2.2.1.1_202102_PQAD_O3_v2.0
D9	E.U. Copernicus Climate Change Service (2019), C3S_D312b_Lot2 Product Quality Assessment Report, PQAR v1.1, C3S_D312b_Lot2.2.1.2_201905_PQAR_O3_v1.1

Acronyms

Acronym	Definition
ACE	Atmospheric Chemistry Experiment
ALGOM	GOMOS Level2 Algorithm Evolution Studies (ESA-funded project)
BIRA-IASB	Royal Belgian Institute for Space Aeronomy
BUV	Backscattered Ultraviolet
CAMS	Copernicus Atmosphere Monitoring Service
CCI	Climate Change Initiative

CDR	Climate Data Record
CDS	Climate Data Store
CF	Climate and Forecast (Metadata Conventions)
C3S	Copernicus Climate Change Service
DLR	Deutsches Zentrum für Luft- und Raumfahrt (German Aerospace Centre)
ECMWF	European Centre for Medium-Range Weather Forecasts
ECV	Essential Climate Variable
ENVISAT	Environmental Satellite (ESA)
EP	Earth Probe
ERA5	ECMWF Re-Analysis 5
ESA	European Space Agency
EU	European Union
FCDR	Fundamental Climate Data Record
FMI	Finnish Meteorological Institute
FORLI	Fast Optimal/Operational Retrieval on Layers for IASI
FP6	Sixth Framework Programme (EU)
FY	Feng Yun (Chinese satellite)
GAD	Gap Analysis Document
GAIA-CLIM	Gap Analysis for Integrated Atmospheric ECV Climate Monitoring (EU H2020 project)
GAID	Gaps Assessment and Impacts Document
GCOS	Global Climate Observation System
GEOMon	Global Earth Observation and Monitoring (EU FP6 project)
GHG	Greenhouse Gas(es)
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
GTO	GOME-type Total Ozone
HALOE	Halogen Occultation Experiment
H2020	Horizon 2020 (EU research and development programme)
IASB-BIRA	Royal Belgian Institute for Space Aeronomy
IASI	Infrared Atmospheric Sounding Interferometer
IASI-NG	IASI New Generation
ICDR	Intermediate Climate Data Record
IR	InfraRed
KIT	Karlsruhe Institute of Technology
KNMI	Royal Netherlands Meteorological Institute
LATMOS	Laboratoire Atmosphères et Observations Spatiales
LP	Limb Profile/Profiler
L1/L2/L3/L4	Level 1/2/3/4
Metop	Meteorological Operational Platform (EUMETSAT)
MIPAS	Michelson Interferometer for Passive Atmospheric Sounding
MLS	Microwave Limb Sounder
MSR	Multi-Sensor Reanalysis
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)
NOAA	National Oceanic and Atmospheric Administration (USA)
NP	Nadir Profile
OMI	Ozone Monitoring Instrument (aboard EOS-Aura)
OMPS	Ozone Mapping and Profiler Suite
OSIRIS	Optical Spectrograph and InfraRed Imaging System (aboard Odin)
OSSSMOSE	Observing System of Systems Simulator for Multi-missiOn Synergies Exploration
Ozone_cci	ESA Climate Change Initiative ozone project
ppbv	Part per billion volume
RAL	Rutherford Appleton Laboratory
R&D	Research and Development
S5P	Sentinel-5 Precursor mission
SABER	Sounding of the Atmosphere using Broadband Emission Radiometry
SAGE	Stratospheric Aerosol and Gas Experiment
SBUV	Solar Backscatter Ultraviolet Radiometer
SCIAMACHY	Scanning Imaging Absorption Spectrometer for Atmospheric CHartographY (aboard Envisat)
SMART	Specific, measurable, achievable, realistic, and time bound
SMR	Sub-Millimetre Radiometer (aboard Odin)
TC	Total Column
TOMS	Total Ozone Mapping Spectrometer
TRD	Target Requirement Document
TROPOMI	Tropospheric Monitoring Instrument (on board S5P)
UARS	Upper Atmosphere Research Satellite
UiB	University of Bremen
UK	United Kingdom
UNI-HB	University of Bremen
UPMC	Université Pierre et Marie Curie
URD	User Requirements Document
USA	United States of America
UTLS	Upper Troposphere / Lower Stratosphere
UV	UltraViolet
VIS	Visible
WMO	World Meteorological Organization
WOUDC	World Ozone and Ultraviolet Radiation Data Centre (at ECCC) http://www.woudc.org/

General definitions

Climate Data Record (CDR)

A (Thematic) Climate Data Record is derived from a FCDR and closely connected to an ECV but strictly covers one geophysical

	variable, whereas an ECV can encompass several geophysical variables. A (F)CDR can encompass several instruments.
Data Product (or: ECV product)	The geophysical product underlying a (I)CDR, characterized by product definition, product name, processing level, instruments used, processing algorithm (name and version), data provider, and data format.
Data Requirement	A quantitative requirement on spatio-temporal coverage and resolution, uncertainty and stability.
Essential Climate Variable (ECV)	A geophysical variable that is associated with climate variation and change as well as the impact of climate change onto Earth [GCOS-200]. ECVs might encompass a set of CDRs with associated Data Products.
Fundamental Climate Data Record (FCDR)	A well-characterized, long-term data record of, *e.g.*, calibrated radiances, with calibrations sufficient to allow the generation of a Data Product that is accurate and stable, in both space and time, to support climate applications. A FCDR includes the ancillary data used in the calibration [GCOS-200].
Gap	An unfulfilled (Target) User Requirement.
Gap Analysis	The assessment of Gaps, *i.e.*, an assessment of the differences between the (Target) User Requirements and their present-day fulfilment.
GCOS requirements	Quantitative Data Requirements for the ECVs on spatiotemporal resolution, accuracy and stability following the GCOS Implementation Plan, 2016 (GCOS-200) and updated by the latest GCOS Implementation Plan, 2022 (GCOS-244) and associated GCOS ECVs Requirements (GCOS-245). These are Target User requirements.
Interim Climate Data Record (ICDR)	A CDR which is regularly updated with an algorithm/system having maximum consistency to the CDR generation algorithm/system. The update cycle depends on the user requirements [GCOS-200].
Target User Requirement	A technology-aware potentially achievable User Requirement which could be regarded as the long-term development goal for an ECV.

User Requirement	A user need for (aspects of) a Data Product, including Data Requirements, metadata information, analysis tools, data formats, etc.
Level 1	Measured satellite data product: geolocated radiance (spectra)
Level 2	Satellite-derived data product: geolocated geophysical variables. Here: ozone information for each ground-pixel
Level 3	Aggregated satellite data product: gridded geophysical variables Here: Gridded ozone information, e.g., 1°x1° monthly
Level 4	Satellite-derived data product: Here: Assimilated ozone columns
Systematic error	Component of measurement error that in replicate measurements remains constant or varies in a predictable manner. "Systematic error" = "Absolute systematic error" (in contrast to "Relative systematic error").
Relative systematic error	Identical with "Systematic error" but after bias correction (especially important for satellite GHG ECV products).
Bias	Estimate of a systematic measurement error (*JCGM, 2008*).
Precision	The measure of reproducibility or repeatability of the measurement without reference to an international standard so that precision is a measure of the random and not the systematic error. Suitable averaging of the random error can improve the precision of the measurement but does not establish the systematic error of the observation (*CMUG-RBD, 2012*). We quantify precision here with the standard deviation (1-sigma) of the error distribution.
Stability	A term often invoked with respect to long-term records when no absolute standard is available to quantitatively establish the systematic error - the bias defining the time-dependent (or instrument-dependent) difference between the observed quantity and the true value (*CMUG-RBD, 2012*). Stability requirements cover inter-annual error changes. If the change in the average bias from one year to another is larger than the

	defined values, the corresponding product does not meet the stability requirement.
Representativity	How much a measured value represents the value over a grid cell of a model. It is important when comparing with or assimilating in models. Measurements are typically averaged over different horizontal and vertical scales compared to model fields. If the measurements are smaller scale than the model it is important. The sampling strategy can also affect this term (*CMUG-RBD, 2012*).
Threshold requirement	The threshold is the minimum requirement to be met to ensure that data are useful for climate-related applications (*CMUG-RBD, 2012*). Threshold requirements are given for statistical quantities (average and standard deviation of an error distribution) rather than for individual soundings. This means that some sub-ensembles of a dataset can be useful and some others not. Threshold requirements are fully driven by the target application (here regional flux inversions), irrespective of available technology.
Goal requirement	The goal is an ideal requirement above which further improvements are not necessary (*CMUG-RBD, 2012*). This requirement is relative to a given state of the art for the target application. Indeed, the more accurate and precise the satellite data products are, the larger their information content is. However, other errors such as model transport errors do not allow exploiting the additional information content data have if they are more accurate than the specified goal requirement.
Breakthrough requirement	The breakthrough is an intermediate level between the “threshold” and “goal “requirements, which - if achieved - would result in a significant improvement for the targeted application. The breakthrough level may be considered as an optimum, from a cost-benefit point of view when planning or designing observing systems (*CMUG-RBD, 2012*).
Horizontal resolution	Area over which one value of the variable is representative of (*CMUG-RBD, 2012*).
Vertical resolution	Height over which one value of the variable is representative of. Only used for profile data (*CMUG-RBD, 2012*).

Observing Cycle	Temporal frequency at which the measurements are required (*CMUG-RBD, 2012*). In this document also the term “Revisit time” is used. The definition is identical with the definition of “Observing cycle”. Both terms refer to the (average) temporal frequency of observation at a given location.

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Scope of the document

This document provides relevant information on target requirements to users of atmospheric ozone climate data records (CDRs). Atmospheric ozone is one of the Essential Climate Variables (ECVs) defined by the GCOS [D1,D6]. The document summarizes the extent to which the current or foreseeable provision of ozone data products meets or fails to meet user requirements. Unfulfilled user requirements are referred to as 'gaps'.

By definition, any gap analysis includes shortcomings of currently fulfilled user needs. When responding to one or more of the identified gaps, funding agencies should however avoid proposing remedying actions that would compete with present-day activities in such a way as to result in creating new gaps.

The current document is the continuation of the target requirement and gap analysis initiated in March 2018 in the framework of the C3S_312a_Lot4 contract (the original precursor to the current contract), which was the first gap analysis for the ECV Ozone [D4]. Through its successive updates, the document has undergone substantial modifications under the contract C3S_312b_Lot2 [D5] and the current contract C3S2_312a_lot2. The modifications account for the release of new, extended or reprocessed ozone data products as well as recent updates to the GCOS requirements [D7]. It is intended to be an evolving document responding to the community's requirements.

Executive summary

The gap analysis of the currently provided C3S ozone data products is based on user requirements pertaining to ozone climate data records. The user requirements on ozone total column, partial columns and concentration profiles can be traced to GCOS [D1,D7] and ESA Ozone_cci+ [D2]. The ozone profile requirements can be traced back to the ESA *Operoz* study [D3].

The set of gaps presented in this document was compiled using a template for gaps which was filled in by the data product providers to assure *SMART (Specific, measurable, achievable, realistic, and time bound)* proposals for (partial) closure of the identified gaps between user requirements and the status of the current ozone data products in the Climate Data Store. Proposed remedies include improvements upon the currently available ozone data products in terms of quality and/or uncertainty estimates, as well as the extension of existing ozone data products, reprocessing activities and new data products.

The results of the gap analysis are summarized in Table 1 including recommendations on how the service can be improved in the future. The recommendations are, in principle, classified as OPER (operational) or R&D (Research and Development). The latter likely requires funding by bodies outside Copernicus (e.g., ESA via CCI or follow-on or related programmes/projects). Note that in comparison with previous versions of the TRD-GAD, some of the gaps were removed since they have been addressed in the meantime leading to an improvement of the ozone portfolio.

Table 1. List of identified gaps for ozone ECVs

C3S service component covered by the Ozone component of project C3S2_312a_Lot2 (satellite-derived ozone ICDRs / CDRs and related services): **List of identified gaps and recommendations on how to improve on them** *(not ordered by priority)*			
GAP ID	**Type**	**Gap**	**Recommendation**
GAP_ALG_1	R&D	Extension of total ozone and provision of tropical tropospheric ozone data records.	Development, testing and application of improved merging algorithms to include the additional measurements from US sensors in the existing European total and tropical tropospheric ozone data records.
GAP_ALG_2	R&D	Reprocessing of L1 data sets used to improve long-term tropospheric ozone records.	L1 data reprocessing + improved handling of instrumental properties in the retrieval scheme.
GAP_ALG_3	R&D	Ozone profile data with vertical resolution in the lower troposphere and upper troposphere / lower stratosphere.	Increase sensitivity and vertical resolution of ozone profile retrieval schemes in the lower troposphere by extending its wavelength coverage to the visible/near-IR. Global data should be produced from 1995 onwards to investigate links between near-

			surface ozone and surface biophysical quantities indicative of ozone precursor emissions. Combining co-located IR with UV observations would significantly improve vertical resolution in the UTLS.
GAP_ALG_4	R&D	Improvement of ozone profile CDRs in the UTLS region.	Generate a specialized climate data record of ozone profiles for UTLS studies, using as many as possible high-quality dataset.
GAP_ALG_5	R&D	Long-term assimilated nadir ozone profiles.	Correction of retrieved O_3 profiles from different instruments (1979-2018) by comparison with the WOUDC reference ground-truth O_3 profiles + assimilation of the corrected nadir profiles to gridded 3D O_3 fields.
GAP_VAL_1	R&D	Need for improved quantification of representativeness errors in satellite and ground-based CDRs and for their comparison.	Derivation of the sampling / representativeness uncertainty in the comparison of ozonesonde and satellite L-3 data sets and re-interpretation of the validation results.
GAP_INP_1	R&D	Better spectroscopic measurements of ozone absorption lines.	Funding of fundamental research activities by, or at least endorsed through, national and international research programmes.

User needs on the continuation of existing ozone data records and the development of a new space infrastructure for the ECV Ozone could be part of a gap analysis. Although a table listing important initiatives for new missions is provided (Section 3.5), the analysis of future mission initiatives is, however, considered out of the scope of the present document.

The document is divided into three chapters. Chapter 1 describes the ozone data products to which the present document refers. Chapter 2 provides the target user requirements for the ECV Ozone. Chapter 3 provides a gap analysis of the ozone data products, covering gaps in data availability and data quality in the past, present and future that should be addressed partly within and partly outside the C3S framework. Research gaps would need to be addressed by further research activities outside the C3S framework.

1. Product description

In this section we provide an overview of the data products for the ECV Ozone to which the present document applies. The data products are CDRs grouped here in three product groups (sections 1.1, 1.2 and 1.3). For each group a table (Table 2, Table 4, Table 6) specifies the product in terms of a product name, product definition (total column, vertical profile, etc.), processing level and sensor input.

Additionally, per data product, information is provided in Table 3, Table 5 and Table 7 on the processing algorithm (name and version), data provider, time period and coverage. The data delivery format in the Climate Data Store (CDS) is always NetCDF using CF metadata conventions.

The ECV ozone data set includes level-3 products for total ozone, tropospheric ozone columns and ozone profiles from nadir sensors as well as stratospheric ozone profiles from limb and occultation sensors.

Total ozone CDRs are produced from UV backscatter sensors (BUV) as well as from the IASI thermal infrared sensor. The BUV (I)CDRs are based on harmonised level-2 data records generated using a common algorithm (GODFIT-v4) applied to the successive GOME, SCIAMACHY, OMI, GOME-2A/B/C, OMPS and TROPOMI sensors. In addition, a merged monthly mean gridded data set (GTO-ECV) is produced from the same sensors excluding OMPS. Complementing these data, total ozone and tropospheric ozone columns are derived from IASI A/B/C sensors based on the FORLI retrieval algorithm. Finally, the total ozone data package also includes the MSR product, which combines data from virtually all existing sensors assimilated into a level-4 data set covering more than 6 decades.

Ozone profiles are derived from nadir and limb/occultation sensors. Nadir ozone profiling sensors provide measurements with good spatial resolution but coarse vertical sampling (typically 5-10 km) in the 0-50 km altitude range. CDRs are generated from the successive GOME, SCIAMACHY, OMI and GOME2A/B sensors, based on a common retrieval algorithm baseline developed at RAL.

In contrast to nadir product types, limb ozone profiles come with coarse horizontal sampling but high vertical resolution (typically 2-3 km) in the 10-120 km altitude range. The limb profile CDRs are based on so-called Harmonized single instruments (HARMOZ) data sets generated from a range of sensors (OSIRIS, OMPS, ACE, MLS, SABER, SAGE-II, SAGE-III, MIPAS, GOMOS, SCIAMACHY, HALOE). We provide single instrument zonal mean time series in 10° latitude bin, as well as two merged data series, one in the form of long-term zonal means covering the period from 1984 until now, and the second (MEGRIDOP) as a latitude-longitude gridded data product starting in 2001.

1.1 Total and tropospheric column products of the Ozone ECV

Total ozone products have been historically derived from backscatter UV measurements using ozone absorption bands in the Huggins bands (320-345 nm). In this wavelength range, the solar radiation penetrates the atmosphere down to the surface providing good sensitivity to the total integrated column. The CDR and ICDR level-3 data set produced in C3S are based on all sensors providing full spectral coverage in the Huggins bands and allowing for the consistent application of a direct-radiance fitting algorithm, such as that developed for GODFIT-v4 (Lerot et al., 2014). These sensors include ERS-2/GOME, ENVISAT/SCIAMACHY, METOP-A/B/C GOME-2, AURA/OMI, SNPP/OMPS and Sentinel-5 P/TROPOMI and cover the time period from 1995 until now. Next to these level-3 products, the Multi-Sensor Reanalysis (MSR) product provides an extended data set of total ozone covering the full period from 1958 until now. This assimilated level-4 product ingests all existing satellite data sets and, for the period before 1970, when no satellite measurements of ozone were available, ground-based measurements from the Dobson reference network are used.

In addition to backscatter UV data, we also provide ozone column ICDRs based on thermal infrared (TIR) nadir measurements performed using the IASI instruments onboard the 3 successive METOP-A/B/C platforms. TIR measurements are a bit less accurate than UV measurements for total ozone, especially over polar regions (Boynard et al., 2018), however they provide both daytime and nighttime observations and they allow for a separation between the total and the tropospheric column, the latter being defined as the column between 0 and 6 km of altitude.

An overview of the total and tropospheric ozone datasets is given in Table 2, while Table 3 provides more detailed specifications for each of them.

Table 2. An overview of the (I) CDRs for the total and tropospheric columns of the Ozone ECV

Product name	Product type	Variable	Processing level	Sensor input
TC_GOME2A	ICDR	Total ozone	Level-3	GOME-2A
TC_GOME2B	ICDR	Total ozone	Level-3	GOME-2B
TC_GOME2C	ICDR	Total ozone	Level-3	GOME-2C
TC_OMI	ICDR	Total ozone	Level-3	OMI
TC_OMPS	ICDR	Total ozone	Level-3	OMPS
TC_S5P	ICDR	Total ozone	Level-3	S5P/TROPOMI
TTC_IASI-A	ICDR	Total and trop. ozone	Level-3	IASI-A
TTC_IASI-B	ICDR	Total and trop. ozone	Level-3	IASI-B
TTC_IASI-C	ICDR	Total and trop. ozone	Level-3	IASI-C
TC_GTO-ECV	ICDR	Total ozone	Level-3	GOME, SCIAMACHY, GOME-2A, GOME-2B, GOME-2C, OMI, TROPOMI
TC_MSR	ICDR	Total ozone	Level-4	Multi-sensor(*)
TC_GOME	CDR	Total ozone	Level-3	GOME
TC_SCIA	CDR	Total ozone	Level-3	SCIAMACHY

(*) Merged/assimilated product based on GOME, SCIAMACHY, OMI, GOME-2A/B, BUV-Nimbus4, TOMS-Nimbus7, TOMS-EP and SBUV-7, -9, -11, -14, -16, -17, -18, -19. For the earliest part of the time-series (before 1970) ground-based Dobson measurements are used to constrain the assimilation, in the absence of any satellite data set.

Table 3. Specifications of the total and tropospheric column Data Products of the Ozone ECV

Product name	Processing algorithm	Data provider	Time period	Coverage
TC_GOME2A	GODFIT-v4	BIRA / DLR	2007 -	Global
TC_GOME2B	GODFIT-v4	BIRA / DLR	2013 -	Global
TC_GOME2C	GODFIT-v4	BIRA / DLR	2019 -	Global
TC_OMI	GODFIT-v4	BIRA / DLR	2004 -	Global
TC_OMPS	GODFIT-v4	BIRA / DLR	2012 -	Global

TC_S5P	UPAS-OFFL	ESA / DLR	2018 -	Global
TTC_IASI-A	FORLI v20151001	LATMOS	2007 -	Global
TTC_IASI-B	FORLI v20151001	LATMOS	2013 -	Global
TTC_IASI-C	FORLI v20151001	LATMOS	2019 -	Global
TC_GTO-ECV	GTO-ECV v3.2	BIRA / DLR	1995 -	Global
TC_MSR	TMDAM	KNMI	1958 -	Global
TC_GOME	GODFIT-v4	BIRA / DLR	1995 - 2003	Global
TC_SCIA	GODFIT-v4	BIRA / DLR	2002 - 2012	Global

1.2 Nadir profile products of the Ozone ECV

Nadir ozone profiles delivered in C3S are based on the backscatter UV (BUV) technique, which can be applied routinely and with high accuracy to many sensors. This technique was historically pioneered with the series of NASA BUV, SBUV and TOMS instruments and later extended to spectrally resolved sensors such as GOME, SCIAMACHY, OMI and GOME- 2. It is based on the exploitation of the strongly variable ozone absorption around the ozone cutoff spectral region (280-320 nm). Although, like in the TIR spectral range, retrieving tropospheric ozone presents a significant challenge in the UV, tropospheric columns can be directly derived from temperature-dependent spectral structures in the Huggins bands. Data products available in C3S are based on an optimal estimation algorithm developed at RAL, UK (Miles et al., 2015) and consistently applied to the GOME, SCIAMACHY, OMI and GOME-2 A/B sensors (see Table 4 and Table 5).

Table 4. An overview of the (I)CDRs for the nadir profile products of the Ozone ECV

Product name	Product type	Variable	Processing level	Sensor input
NP_GOME2A	ICDR	Ozone profile (nadir)	Level-3	GOME-2A
NP_GOME2B	ICDR	Ozone profile (nadir)	Level-3	GOME-2B
NP_OMI	ICDR	Ozone profile (nadir)	Level-3	OMI
NP_GOME	CDR	Ozone profile (nadir)	Level-3	GOME
NP_SCIA	CDR	Ozone profile (nadir)	Level-3	SCIAMACHY

Table 5. Specifications of the nadir profile Data Products of the Ozone ECV

Product name	Processing algorithm	Data provider	Time period	Coverage
NP_GOME2A	RAL fv0300	RAL / KNMI	2007 -	Global
NP_GOME2B	RAL fv0215	RAL / KNMI	2013 -	Global
NP_OMI	RAL fv0214	RAL / KNMI	2004 -	Global
NP_GOME	RAL fv0301	RAL / KNMI	1995 - 2003	Global
NP_SCIA	RAL fv0214	RAL / KNMI	2002 - 2010	Global

1.3 Limb profile products of the Ozone ECV

Highly resolved information (typically 2-3 km) on the vertical distribution of ozone in the atmosphere can only be derived from space using measurements exploiting the limb geometry either (1) in occultation mode using the sun, the moon or stars as a light source or (2) by measuring the solar radiance scattered by the atmosphere or (3) the radiation directly emitted by the atmosphere at microwave or infrared wavelengths. The data records proposed here combine an extensive set of high-quality limb and occultation sensors covering a time-period suitable for trend evaluation (see Table 6). 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. The limb datasets made available in C3S are based on level-2 data products brokered from expert teams responsible for the operation and data processing of the sensors (see Table 7). These products are quality-assessed and assembled in level-3 products that are formatted and documented in a consistent way. Merged data sets are also generated using de-seasonalized anomalies computed from each individual dataset (see Sofieva et al., 2021, 2023). The main advantage of this approach is that biases due to different sampling patterns (including for example the difference in local time) and instrumental biases are automatically removed, which makes these data ideal for long-term analysis.

Table 6. An overview of the (I)CDRs for the limb profile products of the Ozone ECV

Product name	Product type	Variable	Processing level	Sensor input
LMZ_OSIRIS	ICDR	Ozone profile (limb)	Level-3	OSIRIS
LMZ_OMPS	ICDR	Ozone profile (limb)	Level-3	OMPS
LMZ_ACE	ICDR	Ozone profile (limb)	Level-3	ACE
LMZ_MLS	ICDR	Ozone profile (limb)	Level-3	MLS
LMZ_SABER	ICDR	Ozone profile (limb)	Level-3	SABER
LMZ_SAGE-III	CDR	Ozone profile (limb)	Level-3	SAGE-III
LMZ_MERGED	ICDR	Ozone profile (limb)	Level-3	Multi-sensor(*)
LP_MERGED	ICDR	Ozone profile (limb)	Level-3	Multi-sensor(**)
LMZ_MIPAS	CDR	Ozone profile (limb)	Level-3	MIPAS
LMZ_GOMOS	CDR	Ozone profile (limb)	Level-3	GOMOS
LMZ_SCIA	CDR	Ozone profile (limb)	Level-3	SCIAMACHY
LMZ_SAGE2	CDR	Ozone profile (limb)	Level-3	SAGE-2
LMZ_HALOE	CDR	Ozone profile (limb)	Level-3	HALOE

(*) Monthly zonal mean merged product based on MIPAS, GOMOS, SCIAMACHY, OSIRIS, ACE, OMPS and SAGE-2.
(**) Latitude-longitude gridded merged product based on MIPAS, GOMOS, SCIAMACHY, MLS, OMPS and OSIRIS.

Table 7. Specifications of the limb profile Data Products of the Ozone ECV

Product name	Processing algorithm	Data provider	Time period	Coverage
LMZ_OSIRIS	USask v5.10	USask / UNI-HB / FMI	2001 -	Global
LMZ_OMPS-SASK	USask 2D	Usask / FMI	2012 -	Global
LMZ_OMPS-UB	UBR-IUP v2.0	UNI-HB / FMI	2012 -	Global
LMZ_ACE	UoT v3.5/3.6	UoT / UNI-HB / FMI	2004 -	Global
LMZ_MLS	NASA v4.2	NASA / UNI-HB / FMI	2004 -	Global
LMZ_SABER	NASA v2.0	NASA / UNI-HB / FMI	2002 -	Global
LMZ_SAGE-III	NASA v5.1	NASA / UNI-HB / FMI	2017 -	Global
LMZ_MERGED	FMI v2	FMI	1984 -	Global
LP_MERGED	MEGRIDOP_v1	FMI	2001 -	Global
LMZ_MIPAS	KIT/IAA v7R_O3_240	KIT / UNI-HB / FMI	2005 - 2012	Global
LMZ_GOMOS	ALGOM2s v1	UNI-HB / FMI	2002 - 2011	Global
LMZ_SCIA	UBr v3.5	UNI-HB / FMI	2002 - 2012	Global
LMZ_SAGE2	NASA v7.0	NASA / UNI-HB / FMI	1984 - 2005	Global

LMZ_HALOE	NASA v19	NASA / UNI-HB / FMI	1991 - 2005	Global

2. User Requirements

The user community and applications identified for the ECV Ozone are largely derived from the climate monitoring application requirements defined in the ESA *Operoz* study on operational ozone profile requirements [D3].

Global total ozone levels decreased through the 1980s and early 1990s, by about 2.5% in the global mean; the decrease was most pronounced in the Antarctic (related to the Antarctic ozone hole), noticeable but moderate in the mid-latitudes, with very little ozone change in the tropics (WMO 2014). Since 2000 signs of recovery appear in the ozone profile records.

2.1 General user requirements for all products of the Ozone ECV

Continuation of ozone column and profile climate monitoring is recommended by GCOS [D1,D6] and it is required for the verification of the Montreal Protocol and its amendments and adjustments. Also follow-up limb and/or occultation missions are recommended in the coming decades with expected ozone layer recovery [D1,D6].

The 2022 GCOS ECVs Requirements [D7] distinguishes between Goal (G), Breakthrough (B) and Threshold (T) requirements. Goal and breakthrough requirements correspond to the target and threshold user requirements specified in previous versions of this document. This version of the TRD-GAD implements the 2022 nomenclature. However, since in this contract the assessment of compliancy of ozone products with respect to GCOS requirements is still based on GCOS 2016 [D1], we provide both GCOS 2016 and GCOS 2022 values. Note that the implications of the changes introduced in GCOS 2022 will be evaluated by the validation team in consultation with other consortium members and considered for a follow-up contract. Note finally that in addition to GCOS, also requirements from the Ozone_cci User Requirements Document [D2] are taken into account as well as user requirements derived from the ESA *Operoz* study on operational ozone profile requirements [D3].

User requirements specified in this section are organised according to product types. We distinguish between general requirements (valid for all product types – this section), requirements specific to total and tropospheric ozone products (section 2.2), requirements specific to nadir ozone profile product types (section 2.3) and requirements specific to limb profile products (section 2.4). For ozone profile products, user requirements often vary with the altitude region considered.

REQ-O3-1 The geographic coverage of the ozone data products should be global (incl. polar night).

All data products should be provided with a traceable error budget breakdown.

REQ-O3-2	The ozone data products should be provided with a traceable error budget breakdown.

The update frequency of the ozone data records should preferably be once per day and must not be less than once per week. Up to the middle stratosphere included, the value required by GCOS is more demanding and is of every 4 hours (goal).

REQ-O3-3	The ozone data products should be updated at a daily frequency. For GCOS-2022, temporal resolution and timeliness should be of 1 hour (breakthrough: 1 day), except in the UTLS, middle and upper stratosphere where the goal is 6 hours (breakthrough: 1 day).

User requirements on the Ozone ECV include requirements on the data format. All data products are to be provided using NetCDF. Further requirements relate to the metadata, which follow the Climate and Forecast (CF) metadata conventions.

REQ-O3-4	The ozone data products are to be provided in NetCDF.

2.2 User requirements for total and tropospheric column products of the Ozone ECV

The horizontal resolution of the ozone total and tropospheric columns is of 20 km (goal), with breakthrough values of 100 km and 200 km respectively. GCOS-2022 has more stringent requirements for tropospheric ozone: 5 km (goal) and 20 km (breakthrough).

REQ-O3-TC-1	The horizontal resolution of the ozone total column is of 20 km (goal) with a breakthrough value of 100 km.

REQ-O3-TC-2	The horizontal resolution of the ozone tropospheric column is of 20 km (goal) with a breakthrough value of 200 km. GCOS-2022: 5 km (goal) and 20 km (breakthrough).

The 1-sigma uncertainty of the ozone total and tropospheric columns should be of 2% and 8% respectively (goal), with breakthrough values of 3% and 16% respectively. GCOS-2022 has more stringent requirements for both total and tropospheric columns.

REQ-O3-TC-3	The 1-sigma uncertainty of the ozone total column should be of 2% (goal) with a breakthrough value of 3%. GCOS-2022: 2-sigma uncertainty of 1% (goal) and 2% (breakthrough).

REQ-O3-TC-4	The uncertainty of the ozone tropospheric column should be of 8% (goal) with a breakthrough value of 16%. GCOS-2022: 2-sigma uncertainty of 5% (goal) and 10% (breakthrough).

2.3 User requirements for nadir profile products of the Ozone ECV

The user requirements about spatial resolution and uncertainty of the ozone nadir profiles depend on the atmospheric region envisaged.

Horizontal resolution should be as fine as

- 20 km in the troposphere (goal), with a breakthrough value of 200 km;
- 100 km in the stratosphere (goal), with a breakthrough value of 200 km;
- 200 km in the upper stratosphere and mesosphere (goal), with a breakthrough value of 400 km.

GCOS-2022 has more stringent requirements, and uses slightly different definitions for the relevant atmospheric layers, i.e. troposphere, UTLS and Middle and Upper stratosphere.

REQ-O3-NP-1 The horizontal resolution of the nadir ozone profiles should be as fine as the following as a function of the altitude region.

- Troposphere: 20 km (goal), or 200 km (breakthrough).
- Lower and middle stratosphere: 100 km (goal).
- Upper stratosphere / mesosphere: 200 km (goal).

As a function of the altitude region, GCOS-2022 requires a finer horizontal resolution:

- Troposphere: 1 km (breakthrough: 20 km)
- UTLS: 10 km (breakthrough: 50 km)
- Middle and Upper stratosphere: 20 km (breakthrough: 100 km)

The vertical resolution of the ozone nadir profiles should be as fine as 6 km (or partial columns should be provided). GCOS-2022 requirements are more demanding, with a vertical resolution of 1 km in the troposphere (breakthrough: 3 km), 0.5 km in the UTLS (breakthrough: 1 km) and 1 km in the Middle and Upper stratosphere (breakthrough: 3 km).

REQ-O3-NP-2 The vertical resolution of the nadir ozone profiles should be as fine as 6 km (goal), or partial columns should be provided (breakthrough).

As a function of the altitude region, GCOS-2022 requires a finer vertical resolution:

- Troposphere: 1 km (breakthrough: 3 km)
- UTLS: 0.5 km (breakthrough: 1 km)
- Middle and Upper stratosphere: 1 km (breakthrough: 3 km)

The relative uncertainty (1-sigma) of the ozone nadir profiles should be less than 8% in the troposphere and lower stratosphere (breakthrough: 16%) and less than 4% (breakthrough: 8%) above. The absolute uncertainty should be less than 50 ppbv (breakthrough: 100 ppbv) in the lower and middle stratosphere.
GCOS-2022 provides accuracy requirements given at 2-sigma and in percent. These requirements are more stringent than currently considered.

REQ-O3-NP-3 As a function of the altitude region, the relative uncertainty of the ozone nadir profiles should be less than the following values.

- Troposphere and lower stratosphere: 8% (goal) or 16% (breakthrough).
- Middle and upper stratosphere / mesosphere: 4% (goal) or 8% (breakthrough).

Except in the middle and upper stratosphere, GCOS-2022 requires better accuracies (given at a confidence interval of 2-sigma):

- Troposphere: 2% (breakthrough: 5%)
- UTLS: 2% (breakthrough: 5%)
- Middle and Upper stratosphere: 5% (breakthrough: 10%)

REQ-O3-NP-4 In the lower and middle stratosphere, the absolute uncertainty of the ozone nadir profiles should be less than 50 ppbv (goal) or 100 ppbv (breakthrough).

2.4 User requirements for limb profile products of the Ozone ECV

The user requirements about spatial resolution and uncertainty of the ozone limb profiles also depend on the atmospheric region envisaged.

Along-track sampling should be as fine as

- 100 km in the lower and middle stratosphere, with a breakthrough value of 200 km;
- 200 km in the upper stratosphere and mesosphere, with a breakthrough value of 400 km.

In all these altitude regions, GCOS-2022 has more stringent requirements on horizontal resolution.

REQ-O3-LP-1 The along-track sampling of the limb ozone profiles should be as fine as the following as a function of the altitude region.

- Lower and middle stratosphere: 100 km (goal) or 200 km (breakthrough).
- Upper stratosphere / mesosphere: 200 km.

As a function of the altitude region, GCOS-2022 requires a finer horizontal resolution:

- UTLS: 10 km (breakthrough: 50 km)
- Middle and Upper stratosphere: 20 km (breakthrough: 100 km)

The vertical resolution of the ozone limb profiles should be as fine as 1 km in the lower and middle stratosphere (breakthrough: 2 km) and 2 km in the upper stratosphere and mesosphere (breakthrough: 4 km).

REQ-O3-LP-2 The vertical resolution of the limb ozone profiles should be as fine as the following as a function of the altitude region.

- Lower and middle stratosphere: 1 km (breakthrough: 2 km).
- Upper stratosphere / mesosphere: 2 km (breakthrough: 4 km).

As a function of the altitude region, GCOS-2022 requires a finer vertical resolution:

- UTLS: 0.5 km (breakthrough: 1 km)
- Middle and Upper stratosphere: 1 km (breakthrough: 3 km)

The relative uncertainty of the ozone limb profiles should be less than 8% in the lower stratosphere (breakthrough: 16%) and less than 4% (breakthrough: 8%) above. The absolute uncertainty should be less than 50 ppbv (breakthrough: 100 ppbv) in the lower and middle stratosphere.

REQ-O3-LP-3 As a function of the altitude region, the relative uncertainty of the ozone limb profiles should be less than the following values.

- Lower stratosphere: 8% (breakthrough: 16%).
- Middle and upper stratosphere / mesosphere: 4% (breakthrough: 8%).

Especially in the lower stratosphere (UTLS), GCOS-2022 requires a better accuracy (given at a confidence interval of 2-sigma):

- UTLS: 2% (breakthrough: 5%)
- Middle and Upper stratosphere: 5% (breakthrough: 10%)

REQ-O3-LP-4 In the lower and middle stratosphere, the absolute uncertainty of the ozone limb profiles should be less than 50 ppbv (breakthrough: 100 ppbv).

2.5 Summary of numbered user requirements for the Ozone ECV

Here we provide a list of all numbered requirements in this document (with shortened text), so that it can be used as a reference in other documents assessing the compliance with those requirements. Note that in almost all cases, more stringent requirements are required by the most recent edition (2022) of the GCOS ECVs Requirements [D7]. As already stated in the introduction of this section, the implications of these changes need to be evaluated by the validation team in consultation with other consortium members. More time is needed to come up with possible changes to requirements used in the project.

Table 8. User requirements for the Ozone ECV.

C3S service component covered by the Ozone component of project C3S2_312a_Lot2 (satellite-derived ozone ICDRs / CDRs and related services): **List of target user requirements** *(not ordered by priority)*	
REQ. ID	**Requirement**
REQ-O3-1	The geographic coverage of the ozone data products should be global (incl. polar night).
REQ-O3-2	The stability of the ozone data products should be 1% / decade (breakthrough: 3% / decade).
REQ-O3-3	The ozone data products should be provided with a traceable error budget breakdown.
REQ-O3-4	The ozone data products should be updated at a daily frequency – for GCOS, every 4h, except in the upper stratosphere / mesosphere – (breakthrough: weekly).

REQ-O3-5	The ozone data products are to be provided in NetCDF.
REQ-O3-TC-1	The target horizontal resolution of the ozone total column is of 20 km (breakthrough: 100 km).
REQ-O3-TC-2	The target horizontal resolution of the ozone tropospheric column is of 20 km (breakthrough: 200 km).
REQ-O3-TC-3	The target uncertainty of the ozone total column should be of 2% (breakthrough: 3%).
REQ-O3-TC-4	The target uncertainty of the ozone tropospheric column should be of 8% (breakthrough: 16%).
REQ-O3-NP-1	The horizontal resolution of the nadir ozone profiles should be as fine as the following as a function of the altitude region. • Troposphere: 20 km (breakthrough: 200 km). • Lower and middle stratosphere: 100 km – GCOS: 20 km – (breakthrough: 200 km – GCOS: 50 km). • Upper stratosphere / mesosphere: 200 km – GCOS: 20 km – (breakthrough: 400 km – GCOS: 50 km).
REQ-O3-NP-2	The vertical resolution of the nadir ozone profiles should be as fine as 6 km (target); partial columns should at least be provided (breakthrough). As a function of the altitude region, GCOS requires a finer vertical resolution as follows. • Troposphere: 5 km. • Lower and middle stratosphere: 1 km (breakthrough: 2 km). • Upper stratosphere / mesosphere: 3 km.
REQ-O3-NP-3	As a function of the altitude region, the relative uncertainty of the ozone nadir profiles should be less than the following values. • Troposphere and lower stratosphere: 8% (breakthrough: 16%). • Middle and upper stratosphere / mesosphere: 4% (breakthrough: 8%).
REQ-O3-NP-4	In the lower and middle stratosphere, the absolute uncertainty of the ozone nadir profiles should be less than 50 ppbv (breakthrough: 100 ppbv).
REQ-O3-LP-1	The along-track sampling of the limb ozone profiles should be as fine as the following as a function of the altitude region. • Lower and middle stratosphere: 100 km (breakthrough: 200 km). • Upper stratosphere / mesosphere: 200 km – GCOS: 100 km – (breakthrough: 400 km – GCOS: 200 km).
REQ-O3-LP-2	The vertical resolution of the limb ozone profiles should be as fine as the following as a function of the altitude region. • Lower and middle stratosphere: 1 km (breakthrough: 2 km). • Upper stratosphere / mesosphere: 2 km (breakthrough: 4 km).
REQ-O3-LP-3	As a function of the altitude region, the relative uncertainty of the ozone limb profiles should be less than the following values. • Lower stratosphere: 8% (breakthrough: 16%). • Middle and upper stratosphere / mesosphere: 4% (breakthrough: 8%).
REQ-O3-LP-4	In the lower and middle stratosphere, the absolute uncertainty of the ozone limb profiles should be less than 50 ppbv (breakthrough: 100 ppbv).

3. Gap Analysis

An assessment has been made of the differences between the (Target) User Requirements presented in Section 2 and their current fulfilment. A Gap is here defined as an unfulfilled (Target) User Requirement. For C3S2, gaps are seperated into the following four gap types:

(i) Gaps in the development of processing algorithms (Section 3.1),
(ii) Gaps in the methods for estimating uncertainties (Section 3.2),
(iii) Gaps in the quality and fitness-for-purpose of the CDRs (Section 3.3),
(iv) Knowledge gaps, pointing to scientific research needs (Section 3.4).

To collect a set of *SMART* gaps, *i.e.*, unfulfilled user needs that potentially could be resolved by specific, cost and time bound actions, a gap template form was developed and distributed to data providers of ozone data products. The distributed gap template asked for the specification of the gap with one proposed remedy along several entries, among which we retain the following:

- Gap title
- Gap description
- References (papers, project reports)
- Gap impacts (users impact of not addressing the gap)
- Potential remedy for the gap

The set of gaps that has been identified currently and analysed towards remedies includes:

- Extension of total ozone and provision of tropical tropospheric ozone data records
- Long-term assimilated nadir ozone profiles
- Need for improved quantification of representativeness errors in satellite and ground-based CDRs and for their comparison
- Reprocessing of L1 data sets used to improved long-term tropospheric ozone records
- Ozone profile data with vertical resolution in the lower troposphere and upper troposphere / lower stratosphere
- Improvement of ozone profile CDRs in the UTLS region
- Ozone profile data with vertical resolution in the lower troposphere and upper troposphere / lower stratosphere

These gaps are further analysed in sections 3.1 to 3.4. In addition, some other gaps have been identified, but not yet analysed towards *SMART* envisaged remedies. In section 3.5 we discuss some future opportunities for recently launched instruments measuring ozone and tabulate important planned or proposed satellite missions addressing the ECV Ozone.

Most of the gaps identified in this section are being addressed in the framework of the ESA Ozone_cci+ project.

3.1 Development of processing algorithms

In this section, gaps on data coverage are reported given the historical records of the ECV Ozone and the envisaged data availability for the next 10-15 years.

3.1.1 Extension of total ozone and provision of tropical tropospheric ozone data records (GAP_ALG_1)

Gap Description

The current merged data record (GOME-type Total Ozone Essential Climate Variable) developed in the ESA CCI ozone project and included in the C3S Climate Data Store (CDS) contains global total ozone columns from the European satellite sensors GOME/-2, SCIAMACHY, and OMI. It covers the 22 year period from 1995 to 2017 (Coldewey-Egbers et al., 2015). From the same satellite sensors a harmonized tropical tropospheric ozone data record (1995-2017) was developed in the ESA CCI project (Heue et al., 2016), but this data record is currently not included in C3S-CDS.

Furthermore, measurements of total and tropical tropospheric ozone columns from the US sensors TOMS and SBUV/-2 have been carried out since 1978 (Ziemke et al., 1998; Frith et al., 2017), which would allow an extension of existing C3S merged data records backwards in time.

Gap impact

Users need harmonized tropospheric ozone columns in addition to total ozone data records (starting in 1978 with the US sensors and continuing over the next two decades with additional data from the European Copernicus sensors) to perform long-term trend analysis and an investigation of ozone interannual variability on global and regional scales.

Potential remedy

Preparation of merged tropical tropospheric ozone data record (Heue et al., 2016) for inclusion in the C3S Climate Data Store. Development, testing and application of improved merging algorithms to include the additional measurements from US sensors in the existing European total and tropical tropospheric ozone data records.

Underlying close-to-fulfilled but improvable target user requirements:

REQ-O3-1
REQ-O3-2
REQ-O3-TC-3

Underlying unfulfilled target user requirement:

REQ-O3-TC-4

GAP.ID	Type	Gap	Recommendation
GAP_ALG_1	R&D	Extension of total ozone and provision of tropical tropospheric ozone data records.	Development, testing and application of improved merging algorithms to include the additional measurements from US sensors in the existing European total and tropical tropospheric ozone data records.

3.1.2 Long-term assimilated nadir ozone profiles (GAP_ALG_5)

Gap Description

Currently several long-term time series of about 40 years exist for total ozone columns, but no profile information is included. On the other hand, several data sets exist of retrieved ozone profiles in nadir from SBUV in the past till OMI and GOME-2 recently. What is missing is a consistent long time series (40 years), that is intercalibrated between instruments and gridded in time and place. Ideally this should be in time steps of less than 1 day to monitor the diurnal cycle.

Gap impact

Climate modelers have no verification of long-term changes in the vertical distribution in their model. Trends in tropospheric ozone or other altitudes cannot be monitored.

Potential remedy

Step 1
Correct retrieved ozone profiles from different instruments (1979-2018) by comparison with the reference ground-truth ozone profiles of the WOUDC.

Step 2
Data assimilation of the corrected nadir ozone profiles to gridded 3D ozone fields.

Underlying unfulfilled target user requirements:

REQ-O3-NP-3
REQ-O3-NP-4

GAP.ID	Type	Gap	Recommendation
GAP_ALG_5	R&D	Long-term assimilated nadir ozone profiles.	Correction of retrieved O_3 profiles from different instruments (1979-2018) by comparison with the WOUDC reference ground-

	truth O_3 profiles + assimilation of the corrected nadir profiles to gridded 3D O_3 fields.

3.2 Methods for estimating uncertainties

In this section gaps are reported which are relevant to methods for (better) estimating uncertainties, e.g. to enhance knowledge about error characterization and error chains (traceability).

3.2.1 Need for improved quantification of representativeness errors in satellite and ground-based CDRs and for their comparison (GAP_VAL_1)

<u>Gap Description</u>

The vertical column and distribution of atmospheric ozone is measured through several observation techniques from space (*e.g.*, nadir backscatter, solar occultation, limb emission and scattering from different orbits) and from the ground. Differences in spatiotemporal sampling between satellite-based observations, and also between satellite- and ground-based observations, are considerable. Those differences can result in significant uncertainties in monthly data in synoptic-scale grid cells and, especially, in zonal bands. Those so-called sampling/representativeness uncertainties add to, and in several cases, even dominate over the measurement and retrieval uncertainties associated with the individual datasets [D8]. If neglected, these can hamper the ground-based quality assessment of satellite gridded CDRs and, consequently, the C3S ozone profile data validation reported in the PQAR v1 [D9].

Initial estimates of sampling/representativeness uncertainty have been published for some satellite ozone profile data (Sofieva et al., 2014; Millán et al., 2016) and for ground-based total column ozone data (Verhoelst et al., 2015; Coldewey-Egbers et al., 2015). Unfortunately, such estimates have not been reported for ground-based profile observations and for other types of satellite observations. This lack of knowledge was also identified as an important gap in the ground-based capabilities for C3S data validation in the H2020 GAIA-CLIM GAID (gap G3.05). An appropriate quantification and characterization of ground-based sampling errors (systematic component, cycles, noise) is a prerequisite to a more robust and a more detailed assessment of uncertainties in satellite level-3 profile data records.

<u>Gap Impact</u>

As long as sampling/representativeness uncertainties remain unquantified and, hence, neglected in the uncertainty budget of a gridded data product and also in a ground-based evaluations process, they result in:

- A less robust characterization of systematic error and random uncertainty of satellite profile data products, and a lack of knowledge of their pattern in time and space (e.g., cycles and drifts as an evolution of the systematic error);

- A reduced spatiotemporal coverage (e.g., 1990s vs 2000s, Northern mid-latitude vs Tropics and Southern Hemisphere) and scale (e.g., synoptic/zonal, monthly/seasonal/annual) over which quality indicators on CDRs can be derived.

Potential remedy

Step 1

Use of the OSSSMOSE simulator (Observing System of Systems Simulator for Multi-missiOn Synergies Exploration, Verhoelst et al., 2015) to construct model-based simulations of averaged ozone profile data at the spatiotemporal granularity: (1) of an idealized, perfectly sampled (i.e. complete and homogeneous w.r.t the spatiotemporal scales of natural variability) data record; (2) of current gridded C3S satellite data products; and (3) of ozonesonde-based level-3 data records used as ground-based reference. Inclusion in these simulations of the spatiotemporal smoothing properties of the individual measurements as these determine the spatiotemporal representativeness of the individual measurements (Vandenbussche et al., 2011).

Step 2

From these simulations, an analysis and characterisation of the systematic and other component of sampling/representativeness errors in the spatial and temporal domain, including cycles and long-term evolution such as that induced by orbital drift or changes in sampling pattern (see also Damadeo et al., 2018 for the impact of sampling variations due to orbital drift on trend studies). This characterization is to be performed for both the ground-based and the satellite gridded data records, with a focus on those products expected to suffer most from poor underlying spatiotemporal sampling, such as those based on occultation sounders (ACE-FTS, SAGE-II, HALOE, GOMOS).

Step 3

Derivation of the sampling/representativeness uncertainty in the comparison of ozonesonde and satellite level-3 data sets and re-interpretation of the validation results as presented in the C3S PQAR [9] now taking into account the quantitative estimates of sampling difference uncertainty.

Underlying unfulfilled target user requirements:

REQ-O3-NP-3
REQ-O3-NP-4
REQ-O3-LP-3
REQ-O3-LP-4

GAP.ID	Type	Gap	Recommendation
GAP_VAL_1	R&D	Need for improved quantification of representativeness errors in satellite and ground-based CDRs and for their comparison.	Derivation of the sampling/representativeness uncertainty in the comparison of ozonesonde and satellite L-3 data sets and re-interpretation of the validation results.

3.3 Opportunities to improve quality and fitness-for-purpose of the CDRs

In this section gaps are reported which are relevant to the quality of the data products. Activities in the research domain could feed into gap remedies for C3S. One gap w.r.t. (tropospheric) ozone has been identified but not yet analyzed in detail (section 3.4.1). A second gap that has been identified and analyzed relates to the improvement of ozone profiles in the polar regions (3.4.2).

3.3.1 Reprocessing of L1 data sets used to improved long-term tropospheric ozone records (GAP_ALG_2)

Gap Description

Significant new information on GOME-1 and -2A/-2B/-2C pre-flight and inflight calibration is emerging, which will benefit production of new "Level-1" mission data sets. Accounting for instrumental artefacts to the level required for reliable multi-year, global data sets is likely to require further R&D, especially with respect to tropospheric ozone.

Potential remedy

Activities would encompass reprocessed L1 data sets and improved handling of instrumental properties in the retrieval scheme.

Underlying unfulfilled target user requirement:

REQ-O3-TC-4

GAP.ID	Type	Gap	Recommendation
GAP_ALG_2	R&D	Reprocessing of L1 data sets used to improve long-term tropospheric ozone records.	L1 data reprocessing + improved handling of instrumental properties in the retrieval scheme.

3.3.2 Ozone profile data with vertical resolution in the lower troposphere and upper troposphere / lower stratosphere (GAP_ALG_3)

Gap Description

The complex role played by atmospheric ozone in the evolving Earth system is critically dependent upon its vertical profile as well as its geographical distribution. The value of multi-year global satellite data to Earth system science is therefore critically dependent upon vertical resolution. Global height-resolved ozone distributions spanning the troposphere and stratosphere from 1995 onwards have been produced from a series of UV nadir-sounders within ESA CCI, with the ozone profile retrieval scheme developed by RAL. This scheme is considered state-of-the-art in regard to its tropospheric ozone sensitivity, however, vertical resolution in the lower troposphere and in the upper troposphere / lower stratosphere (UTLS) achievable by UV sounding alone is fundamentally limited by atmospheric radiative transfer. Vertical resolution in these two important height regions therefore limits the potential value of these data to Earth system science; particularly ozone-biosphere feedbacks (mediated through surface ozone deposition via plant uptake) and ozone radiative forcing (for which sensitivity greatest in the UTLS).

Gap impact

The data record from European nadir-UV sounders extends back to 1995 and is continuous. However, because their vertical resolution is limited in both the lower troposphere and the UTLS, the value of data produced for ESA CCI, and now C3S, is limited in these key respects for Earth system science (*e.g.*, ozone-biosphere links, composition – climate links) and other applications, *e.g.*, air quality. The potential of Europe's nadir-UV sounders has therefore yet to be fully realised through data available for users. Future scientific studies and international assessments (*e.g.*, IPCC, WMO) will therefore benefit less from European satellites than they would do if this gap could be closed.

Potential remedy

By extending wavelength coverage of the RAL uv-only retrieval scheme to visible/near-IR, its sensitivity and vertical resolution will be substantially increased in the lower troposphere. Global data will be produced from 1995 onwards to investigate links between near-surface ozone and surface biophysical quantities indicative of plant health, air quality and ozone precursor emissions. By combining co-located IR with UV observations, vertical resolution would be significantly improved in the UTLS. Typically, a single layer (~6-20 km) can be fully-resolved by UV-only, whereas multiple layers can be independently retrieved by adding IR.

(Part 1) Extension from UV to VIS/near-IR

Substantial preparatory R&D has already been performed in the frame of the UK NERC National Centre for Earth Observation (NCEO) to simulate the addition of VIS/IR spectral to UV coverage for ozone profile retrieval and to demonstrate with real flight data the necessary consistency between height-integrated ozone columns retrieved from UV and visible bands. Further R&D is required to optimise spectral coverage along with representation of surface biophysical, atmospheric and instrumental variables and prior constraints for the VIS/near-IR step. Attention will be given to extending coverage to longer UV wavelengths as well as to the visible and near-IR ozone bands. The scheme will be demonstrated and value added by the VIS/NIR extension quantified through comparison of UV-only and UV/VIS/NIR with ozonesondes, CAMS re-analysis and the surface in situ network.

(Part 2) Combination with co-located IR

A scheme to retrieve height-resolved ozone from the IR nadir-sounder IASI has been developed and applied in the frame of NERC's NCEO to the full Metop-A mission. R&D is required to further refine the IR scheme and to optimise use of co-located IASI (IR) and GOME-2 (UV) information in a combined retrieval on the sunlit side of the orbit. The scheme will be demonstrated with the full Metop-A mission and the value of the combined retrieval quantified by assessment against stand-alone GOME-2 and IASI retrievals in comparison with ozonesondes, surface in situ networks and CAMS re-analyses.

Underlying partly unfulfilled target user requirement:

REQ-O3-NP-2

GAP.ID	Type	Gap	Recommendation
GAP_ALG_3	R&D	Ozone profile data with vertical resolution in the lower troposphere and upper troposphere / lower stratosphere.	Increase sensitivity and vertical resolution of RAL retrieval scheme in the lower troposphere by extending its wavelength coverage to the visible/near-IR. Global data will be produced from 1995 onwards to investigate links between near-surface ozone and surface biophysical quantities indicative of ozone precursor emissions. Combining co-located IR with UV observations would significantly improve vertical resolution in the UTLS.

3.3.3 Improvement of ozone profile CDRs in the UTLS region (GAP_ALG_4)

Gap Description

The upper troposphere and the lower stratosphere are difficult to explore from space. Nadir-viewing instruments do not have sufficient vertical resolution, while the retrievals from limb-viewing satellite measurements in the UTLS are challenging due to presence of clouds, lower signal-to-noise ratio and a strong gradient of species across the tropopause. The satellite data in the UTLS have rather substantial biases with respect to each other and different representation of natural cycles as a result of different sampling patterns and the specifics of retrieval algorithms (Sofieva et al., 2015). Currently, the trends in the UTLS under intensive investigation; the trend estimates from different merged satellite datasets can differ significantly (Steinbrecht et al., 2017).

In the framework of the Ozone_cci+ project, a long-term ozone profile climate data record (1984-present) for stratospheric trend analyses has been created, in which the data from 9 satellite instruments (SAGE II, OSIRIS, GOMOS, MIPAS, SCIAMACHY, ACE-FTS, OMPS-LP, SAGE-III/ISS, POAM-III/SPOT) are merged (Sofieva et al., 2017). The merging method, which makes use of the de-seasonalized anomalies, seems to be optimal also for the UTLS, as it automatically removes biases. The trends in the UTLS estimated using the merged SAGE–CCI–OMPS+ data follow the expected trend.

The SAGE-CCI-OMPS+ dataset has been created mainly for ozone trend studies in the stratosphere, therefore it is not fully optimized for the trend analyses in the UTLS. For UTLS studies, the dataset can be enhanced by using also the data from MLS/Aura. It is expected that inclusion of MLS would improve the data quality and stability.

Gap Impact

The reliable datasets for studies trends in the UTLS are of high importance, because dynamical, chemical and radiative coupling between the stratosphere and troposphere are among the important processes that must be understood for prediction of global trends. In addition, a reliable ozone profile CDR in the UTLS is important for climate model validation.

Potential remedy

We propose the production of a specialized ozone profiles climate data record for the UTLS studies. In order to create a good climate data record, it is important to use as many as possible high-quality datasets. For the UTLS studies, the SAGE-CCI-OMPS+ dataset can be enhanced by using the data from Microwave Limb Souder on the Aura satellite.

While for the trend studies in the upper stratosphere, the conversion of ozone profiles to other units might introduce additional uncertainty (MLS retrieves ozone mixing ratio of pressure grid, while Ozone_cci instruments give number density profiles on altitude grid), this should not be a problem in the UTLS. We propose to include MLS data into the merged dataset. In addition, the merging method described in Sofieva et al., (2017) will be compared with alternative merging methods by Ball et al., (2017). Extensive inter-comparisons of satellite and ground-based data will be performed.

Underlying unfulfilled target user requirements:

REQ-O3-LP-3
REQ-O3-LP-4

GAP.ID	Type	Gap	Recommendation
GAP_ALG_4	R&D	Improvement of ozone profile CDRs in the UTLS region.	Generate a specialized climate data record of ozone profiles for UTLS studies, using as many as possible high-quality datasets. The SAGE-CCI-OMPS+ dataset can be enhanced by using Aura/MLS data.

3.4 Scientific research needs

Gaps which are pure knowledge gaps would require fundamental research activities. One could think of, *e.g.*, better spectroscopic measurements of ozone absorption lines. Funding of scientific research activities by, or at least endorsed through, national and international research programmes would be most suited to fill fundamental knowledge gaps. Also, universities could play an important role to explore unknown territories with respect to the ECV Ozone.

Underlying fulfilled but improvable target user requirement:

REQ-O3-3

GAP.ID	Type	Gap	Recommendation
GAP_INP_1	R&D	Better spectroscopic measurements of ozone absorption lines.	Funding of fundamental research activities by, or at least endorsed through, national and international research programmes.

So far, no specific knowledge gaps requiring scientific research have been reported for the present-day ozone data records. However, a lack of identified gaps does not imply that such gaps may not appear for the ECV Ozone in the future. The identification of important knowledge gaps related to the ozone products provided in the CDS is an ongoing effort by the research community.

3.5 Opportunities to exploit the Sentinels and any other relevant satellite

In this section any new opportunities arising from recently launched, planned and proposed future missions for the ECV Ozone are indicated. In particular the Copernicus atmospheric Sentinels 4 and 5 to be launched by late 2024 - early 2025 are of particular relevance.

Recently launched satellite instruments targeting ozone include:

- GIIRS[1] (Geostationary Interferometric Infrared Sounder) on Feng-Yun FY-4A (2017-2021) and FY-4B (2019-2024)
- SAGE III on ISS [2] (2017)
- TROPOMI[3] on Sentinel-5p (2017)
- OMPS[4] on JPSS-1 (2017) and JPSS-2 (2022)

Some of these datasets (SAGE-III on ISS and S5P/TROPOMI) have already been integrated in the current version of the ozone portfolio. In the future, more activities will have to be defined to transform the recent and upcoming data products into long-term ozone data records.

Further to the recently launched instruments, additional missions carrying instruments targeting ozone have been either proposed or are planned. A list of the planned upcoming missions is included in Table 9 below. Note that planned missions targeting ozone from using limb-emission using either IR and/or mm-wave spectral range are lacking for the 2020-2030 timeframe.

[1] https://fy4.nsmc.org.cn/nsmc/en/instrument/GIIRS.html
[2] https://sage.nasa.gov/missions/about-sage-iii-on-iss/
[3] http://www.tropomi.eu/
[4] https://www.star.nesdis.noaa.gov/jpss/OMPS.php

Table 9. Planned and proposed satellite missions targeting ozone

Mission	Time coverage (Estimated start year + ...)	Instruments (viewing direction)
Planned missions		
MTG-S1[5]	2025+	IRS (nadir), Sentinel-4 (nadir)
Metop_SG[6]	2025+	IASI-NG (nadir); Sentinel-5 (nadir)
Altius[7]	2026+	Altius (solar occultation limb)
Proposed missions		
FY-4MW & FY-4D[8]	2024+	MWIR (Mid-Wave Infrared)/TIR (Thermal Infrared)
CAIRT[9], ESA Explorer-11	2028+	(solar occultation, limb)

3.6 Summary of numbered gaps for the Ozone ECV

Here we provide a list of all numbered gaps in this document (with shortened text). Note that some of those gaps are being addressed as part of the ongoing ESA Ozone_cci+ project[10].

Table 10. Gaps for the Ozone ECV.

C3S service component covered by the Ozone component of project C3S2_312a_Lot2 (satellite-derived ozone ICDRs / CDRs and related services): **List of gaps**		
GAP ID	**Gap description**	**Recommendation**
GAP_ALG_1	*Extension of total ozone and provision of tropical tropospheric ozone data records.	Development, testing and application of improved merging algorithms to include the additional measurements from US sensors in the existing European total and tropical tropospheric ozone data records.
GAP_ALG_2	Reprocessing of L1 data sets used to improved long-term tropospheric ozone records.	L1 data reprocessing + improved handling of instrumental properties in the retrieval scheme.
GAP_ALG_3	*Ozone profile data with vertical resolution in the lower	Increase sensitivity and vertical resolution of RAL retrieval scheme in the lower troposphere

[5] https://www.eumetsat.int/meteosat-third-generation
[6] https://www.eumetsat.int/metop-sg
[7] https://www.esa.int/Applications/Observing_the_Earth/Altius
[8] https://fy4.nsmc.org.cn/nsmc/en/satellite/FY4.html
[9] https://www.sparc-climate.org/2021/06/25/cairt-mission-proposal-selected-to-compete-for-earth-explorer-11-call-for-membership-to-the-mission-advisory-group/
[10] https://climate.esa.int/en/projects/ozone/about/

	troposphere and upper troposphere / lower stratosphere.	by extending its wavelength coverage to the visible/near-IR. Global data will be produced from 1995 onwards to investigate links between near-surface ozone and surface biophysical quantities indicative of ozone precursor emissions. Combining co-located IR with UV observations would significantly improve vertical resolution in the UTLS.
GAP_ALG_4	Improvement of ozone profile CDRs in the UTLS region.	Generate a specialized climate data record of ozone profiles for UTLS studies, using as many as possible high-quality datasets. The SAGE-CCI-OMPS+ dataset can be enhanced by using Aura/MLS data.
GAP_ALG_5	Long-term assimilated nadir ozone profiles.	Correction of retrieved O_3 profiles from different instruments (1979-2018) by comparison with the WOUDC reference ground-truth O_3 profiles + assimilation of the corrected nadir profiles to gridded 3D O_3 fields.
GAP_VAL_1	*Need for improved quantification of representativeness errors in satellite and ground-based CDRs and for their comparison.	Derivation of the sampling/representativeness uncertainty in the comparison of ozonesonde and satellite L-3 data sets and re-interpretation of the validation results.
GAP_INP_1	Better spectroscopic measurements of ozone absorption lines.	Funding of fundamental research activities by, or at least endorsed through, national and international research programmes.

*Gap addressed at least in part in the framework of the ESA Ozone_cci+ project

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