Ozone_cci+

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DOCUMENT CHANGE RECORD

Issue	Revision	Date	Modified items
0	4.5	11/02/2011	Draft version submitted to CMUG and ESA for comments
1	0	11/04/2011	- Tables reformatted to fit on one page - Explanation why a few years of limb data are already worthwile - Added radiative forcing in tables (remark CMUG) - Added data assimilation application for Level-2 data (remark CMUG) - Added that requirement tables are for Level-2 and that aggregated level-3 products should not be homogenized/degraded to the instrument which the lowest accuracy over the targeted time period (remark CMUG) - Changed the targeted vertical resolution requirement for the nadir instruments in UTLS to 3-6 km (from 1-3 km) with argument that nadir has better horizontal coverage and add request for assimilated product from the nadir instruments to improve upon vert. resolution esp in the UTLS region. The requirements implicitly include capabilities of TIR sounders. (remark CMUG) - data requirements tables added
1	1	29/04/2011	Final version approved by ESA
2	0	15/06/2011	Revised according to preliminary remarks from CMUG
2	1	21/11/2011	Revised according to final remarks from CMUG
2	2	18/09/2014	Start Document for Phase 2
3	0	11/03/2016	Revisions Phase-2; ozone profile requirements aligned with the final report of the ESA Operoz study (2015) and a few minor text updates

3	1	05/03/2021	Updates in Sections 3.1 and Section 6 in reference to (proposed) updates in the GCOS requirements for ozone products; Section 3.4 removed (obsolete); some minor revisions
4	0	18/04/2024	Updated GCOS-245 (2022) ECV requirements, taken from the WMO Oscar database in March 2024. Minor changes w.r.t user and data requirements for the tropospheric ozone products, in line with the products described in PSD v6.0. A more detailed discussion on cross ECV requirements for climate model process evaluations (Section 2.4).
4	1	26/03/2025	Update of Fig. 1.

Executive Summary

This User Requirements Document (URD) describes the user requirements for the total ozone column products, tropospheric ozone products, as well as nadir- and limb-based vertical profile ozone products developed and delivered through the Ozone_cci+ project. In Phase 2 of this project (2022-2024) the tropospheric ozone products were reintroduced. This URD v4.1 is similar in content to earlier versions of the URD and mainly expands on the tropospheric ozone user needs. The user requirements as described during earlier phases of the project are integrally incorporated.

Information in this URD is directly linked to the detailed specifications of the Ozone_cci+ ozone products in the Product Specification Document (PSD) and the Product User Guide (PUG). These products details are not repeated here.

This URD document

- specifies the user requirements in terms of
    - geophysical variables and their associated uncertainties;
    - definition of the variable names and their meanings;
    - resolution and spatio-temporal sampling and coverage;
    - ancillary output requirements including formats and metadata content;
- refers to user requirements on ozone products put forward by other international collaboration frameworks, preliminary WMO/GCOS;
- provides a rationale for the user requirements from a modelling perspective.

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1 Introduction

1.1 Purpose

This User Requirements Document (URD) of the ESA Ozone_cci+ project summarises the user requirements for four ozone ECV (Essential Climate Variable) products: total ozone columns, tropospheric ozone, nadir-based ozone profiles, and limb-based ozone profiles. Any ECV is generally based on an intermediate dataset called a "Fundamental Climate Data Record" (FCDR) defined as follows: An FCDR denotes a long-term data record, involving a series of instruments, with potentially changing measurement approaches, but with overlaps and calibrations sufficient to allow the generation of homogeneous products providing a measure of the intended variable that is accurate and stable enough for climate monitoring. FCDRs include the ancillary data used to calibrate them. This document is established consisting of a complete, structured set of individual end-user requirements for the four ozone ECV products and the FCDRs required to achieve them.

The user requirements in this document are based on the ozone requirements of GCOS (GCOS-92; GCSO-107; GCOS-138; GCOS-143; GCOS-244 and GCOS-245), the CMUG, IGACO (2004), and the WMO rolling requirements (WMO, 2024). The first consolidated version of this URD (v1.1) was published in 2011. An important update was produced during Ozone_cci Phase-2 (URD v3.0, 2016) to provide a refinement of the ozone profile requirements for long-term monitoring which aligned with the final report of the *Operoz* study for ESA on 'User requirements for monitoring of stratospheric ozone at high vertical resolution; Operoz: Operational ozone observations using limb geometry' (ESA, 2015).

In 2019/2020, an open consultation by the World Meteorological Organization (WMO) on ECV requirements was started. Subsequently an ad-hoc group of experts has been working on the observational requirements for the ozone ECV. Based on the user input and discussions in this group, URD version 3.1 (March 2021) listed slightly revised and newly proposed GCOS requirements pre-empting on updated GCOS requirements were.

In version 4.0 (March 2024) the consolidated GCOS requirements are included for all ozone product types (GCOS-245). Moreover, the tropospheric ozone user and data requirements were further explained in support of the product development of tropospheric ozone climate data records.

The scientific rationale behind the selection of the Ozone_cci data products and the provided requirements is given as appropriate without implying a complete justification.

1.2 Scope

The scope of the URD is defined in relation to other project documents, including the Product Specification Document (PSD). The user requirements include per product type (total column, tropospheric ozone, nadir ozone profile, and limb ozone profile) the quantitative ozone data requirements, including (total) uncertainty, spatial resolution, observation frequency, time period, and overall stability. It also includes a clarification (rationale) for the given requirements for traceability. Specific data product requirements with respect to e.g. data format and specific error specifications are given in full detail in the PSD for the respective level-2, level-3 and level-4 ozone data products.

In Chapter 2, we describe the various existing requirements on ozone products for climate research, especially the requirements from GCOS and CMUG. Chapter 3 introduces the scientific rationale for the Ozone_cci+ products and in Chapter 4, the user requirements, their rationale and traceability are presented.

1.3 Applicable documents

CMUG, 2010: Requirement Baseline Document, Deliverable 1.2, Climate Modelling User Group, version 1.3, November 2010

ESA, 2015: User requirements for monitoring the evolution of stratospheric ozone at high vertical resolution; Operoz: Operational ozone observations using limb geometry. Eds. van Weele, M., R. Müller, M. Riese, R. Engelen, M. Parrington, V.-H. Peuch, M. Weber, A. Rozanov, B. Kerridge, A. Waterfall, and J. Reburn (ESA Contract 4000112948/14/NL/JK)

GCOS-92, 2004: Implementation plan for the global observing system for climate in support of the UNFCCC, composed by World Meteorological Organization, Intergovernmental Oceanographic Commission, United Nations Environment Programme, and International Council for Science, October 2004, (WMO-TD No. 1219)

GCOS-107, 2006: Systematic observation requirements for satellite-based products for Climate, GCOS – 107, composed by World Meteorological Organization and Intergovernmental Oceanographic Commission, September 2006, (WMO-TD No. 1338)

GCOS-138, 2010: Implementation plan for the global observing system for climate in support of the UNFCCC (2010 update), composed by World Meteorological Organization, Intergovernmental Oceanographic Commission, United Nations Environment Programme, and International Council for Science, August 2010, (GOOS-184, GTOS-76, WMO-TD No. 1523)

GCOS-143, 2010: Guideline for the Generation of Datasets and Products Meeting GCOS Requirements, (WMO-TD No. 1530)

GCOS-244, 2022: The 2022 GCOS Implementation Plan, composed by World Meteorological Organization (WMO); United Nations Environment Programme (UNEP); International Science Council (ISC); Intergovernmental Oceanographic Commission of the United Nations Educational, Scientific and Cultural Organization (IOC-UNESCO), 2022, https://library.wmo.int/idurl/4/58104

GCOS-245, 2022: The 2022 GCOS ECV Requirements, composed by World Meteorological Organization (WMO); United Nations Environment Programme (UNEP); International Science Council (ISC); Intergovernmental Oceanographic Commission of the United Nations Educational, Scientific and Cultural Organization (IOC-UNESCO), 2022, https://library.wmo.int/idurl/4/58111

IGACO, 2004: The changing atmosphere. An integrated global atmospheric chemistry observation theme for the IGOS partnership. Report of the Integrated Global Atmospheric Chemistry Observation (IGACO) theme team, September 2004 (ESA SP-1282, GAW No. 159, WMO-TD No. 1235)

World Meteorological Organization (WMO), 2022, Scientific Assessment of Ozone Depletion: 2022, GAW Report No. 278, 509 pp., WMO, Geneva.

World Meteorological Organization (WMO), 2024, OSCAR (Observing Systems Capability Analysis and Review Tool, https://www.wmo-sat.info/oscar/observingrequirements (latest access, March 2024)

2 Overview of Ozone requirements

2.1 Global Climate Observing System (GCOS)

The goal of the **Global Climate Observing System** (GCOS) is to provide continuous, reliable, comprehensive data and information on the state and behaviour of the global climate system. The aims of GCOS which are directly related to *Ozone_cci* are (1) monitoring the climate system, (2) detecting and attributing climate change, and (3) assessing impacts of, and supporting adaptation to, climate variability and change.

Essential climate variables (ECVs) are required to improve our understanding of the climate system. In conjunction with numerical modelling they support hindcasts and projections of the climate system. In the context of Ozone_cci, a better understanding of natural and anthropogenic forcings affecting the atmospheric ozone distribution and ozone-climate interactions will be aimed for through the development of Fundamental Climate Data Records (FCDRs) for ozone. Numerical models, in particular Chemistry-Climate Models (CCMs) are valuable tools to improve our knowledge about dynamical, physical and chemical processes in the atmosphere and feedback mechanisms, and how they are influenced in the future by climate change.

In addition to climate requirements, observations of most of the ECVs have many more important application areas: for example, all standard meteorological variables are fundamental to support numerical weather forecasting; tropospheric ozone, aerosols, and their precursors are important for air quality; vegetation and land-usage maps are used for forestry and ecological/biodiversity assessments. Each application has differing uncertainty and spatial/temporal resolution requirements but an appropriately sustained composite observing system for all ECVs could be a major response to the needs of all GEOSS applications and Societal Benefit Areas including Climate.

Through the development of a set of satellite-based ozone FCDRs Ozone_cci provides a significant contribution to GCOS. Long-term consolidated ozone data sets based on different satellite instruments are the foundation for improved model quality evaluation, allowing a more detailed insight into individual dynamical and chemical processes. For example, global information derived from satellite instruments about the vertical distribution of ozone and its short- and long-term variability is patchy and contains large uncertainties.

Long-term consolidated data sets are mainly required for: (1) Monitoring the Earth climate system on longer (decadal) time scales; (2) Investigation of long-term changes as well as of short-term variability; (3) Improved description of processes in numerical models for more robust assessment of future evolution.

The GCOS requirements for horizontal and vertical resolution and observation cycle are mainly justified by the commonly used (standard) resolution of currently available and used model systems (e.g. Morgenstern et al., 2010; 2017, for the CCMs). For the troposphere, regional models are often used which have a much higher horizontal resolution.

The GCOS user requirements for uncertainty is a 2-sigma requirement for closeness of agreement between product values and true values. As true values are unknown, users are provided in practice with product values that are estimates of true values, and producers may also provide estimates of the uncertainties of their product values.

For example, a monthly-mean ozone data set (mixing ratios) on a horizontal 2° x 2° grid with a vertical resolution of 2 km covering multiple decades would be an extremely valuable tool for model validation, in particular if metadata is provided like the error in each bin, a quality marker (maybe the number of cloud free measurements used), etc.

GCOS requirements are technology aware though not limited to current observational capabilities. Target requirements ('Goal') might refer to desired requirements for future (operational) observations. This URD however sets achievable user and data requirements for the ozone ECV and FCDRs derived from existing observations (and with known attributes) of the past 30 years, as well as including the future targets. The translation of GCOS requirements to practical ozone ECV product requirements is discussed in Section 4 of this URD.

In Table 1, we list the full set of rolling requirements in the OSCAR database of WMO (https://www.wmo-sat.info/oscar/observingrequirements, last accessed: March 2024) in relation to the application area *monitoring of atmospheric composition* and in line with GCOS-245 (2022). The coverage for each ECV product is global unless indicated otherwise. Note that the OSCAR database includes ozone observational requirements also for two other application areas: (i) Providing Atmospheric Composition information to support services in urban and populated areas and (ii) Forecasting of atmospheric composition.

Table 1: The GCOS ozone ECV requirements in the OSCAR database for the application *climate monitoring* (last accessed : March 2024; entree number as indicated per ozone product below). G = Goal; B = Breakthrough; T = Threshold. FT = Free Troposphere; UTLS = Upper Troposphere Lower Stratosphere; MUS = Middle and Upper Stratosphere.

Total Column (no. 802)	**G / B / T**	**Unit**
Horizontal resolution	20 / 100 / 500	km
Vertical resolution	n/a	n/a
Observing cycle	60 min / 24 hrs / 30 days	minutes / hours / days
Timeliness	60 min / 24 hrs / 30 days	minutes / hours / days
Measurement uncertainty	1 / 2 / 3	%
Stability	1 / 2 / 3	% / decade

Stratospheric Column (no. 1015)	G / B / T	Unit
Horizontal resolution	20 / 100 / 500	km
Vertical resolution	n/a	n/a
Observing cycle	60 min / 24 hrs / 30 days	minutes / hours / days
Timeliness	6 hrs / 24 hrs / 30 days	minutes / hours / days
Measurement uncertainty	1 / 3 / 5	%
Stability	1 / 2 / 3	% / decade

Tropospheric Column (no. 1014)	G / B / T	Unit
Horizontal resolution	5 / 20 / 100	km
Vertical resolution	n/a	n/a
Observing cycle	60 min / 6 hrs / 30 days	minutes / hours / days
Timeliness	60 min / 24 hrs / 30 days	minutes / hours / days
Measurement uncertainty	5 / 10 / 15	%
Stability	1 / 2 / 3	% / decade

Mole fraction FT (no. 1010)	G / B / T	Unit
Horizontal resolution	1 / 20 / 100	km
Vertical resolution	1 / 3 / 5	km
Observing cycle	60 min / 6 hrs / 30 days	minutes / hours / days
Timeliness	60 min / 24 hrs / 30 days	minutes / hours / days
Measurement uncertainty	2 / 5 / 10	%
Stability	1 / 2 / 3	% / decade

Mole fraction UTLS (no. 1012)	G / B / T	Unit
Horizontal resolution	10 / 50 / 200	km
Vertical resolution	0.5 / 1 / 3	km
Observing cycle	6 hrs / 24 hrs / 30 days	hours / days
Timeliness	6 hrs / 24 hrs / 30 days	hours / days
Measurement uncertainty	2 / 5 / 10	%
Stability	1 / 2 / 3	% / decade

Mole fraction MUS (no. 1013)	G / B / T	Unit
Horizontal resolution	20 / 100 / 500	km
Vertical resolution	1 / 3 / 10	km
Observing cycle	6 hrs / 24 hrs / 30 days	hours / days
Timeliness	4 hrs / 24 hrs / 30 days	hours / days
Measurement uncertainty	5 / 10 / 15	%
Stability	1 / 2 / 3	% / decade

2.2 Climate Modelling User Group (CMUG)

The main objective of the Climate Modelling User Group (CMUG) is to provide guidelines within ESA's Climate Change Initiative to facilitate the optimal use of the data products produced. In particular, it is necessary to foster the scientific exploitation of global satellite data products for the community of climate modellers and chemistry-climate modellers. The Climate Research Group (CRG) within Ozone_cci refines these user requirements as well as necessary specification for the required data products. They help to integrate and assess the global ozone data products in the context of numerical models. Moreover, they promote and support the use of ozone data products originated from this project.

Table 2: The CMUG requirements on ozone (CMUG, D1.2, version 1.3, November 2010). SSEOB stands for "Single sensor uncertainty estimates for every observation".

Parameter	Application	Horizontal Resolution (km)	Vertical Resolution (km)	Observing Cycle (h)	Precision (%)	Accuracy (%)	Stability (%)	Types of error
Ozone profile								
Higher stratosphere & mesosphere (HS & M)	Model Development and Evaluation	500	3	48	15	15%	3.0 %/decade	SSEOB
	Reanalysis and Data Assimilation	100	1	6	5	5%	1.0 %/decade	SSEOB
Lower stratosphere (LS)	Model Development and Evaluation	100	2	72	15	15%	3.0 %/decade	SSEOB
	Reanalysis and Data Assimilation	75	1	6	5	5%	1.0 %/decade	SSEOB
Higher troposphere (HT)	Model Development and Evaluation	100	2	72	20	20%	3.0 %/decade	SSEOB
	Reanalysis and Data Assimilation	20	1	6	5	5%	1.0 %/decade	SSEOB
Lower troposphere (LT)	Model Development and Evaluation	50	2	72	20	20%	3.0 %/decade	SSEOB
	Reanalysis and Data Assimilation	10	1	3	10	10%	1.0 %/decade	SSEOB
Ozone								
Troposphere column	Model Development and Evaluation	50		72	15	15	5.0 %/decade	SSEOB
	Reanalysis and Data Assimilation	10		3	5	5	3.0 %/decade	SSEOB
Total column	Model Development and Evaluation	50		72	15	15	5.0 %/decade	SSEOB
	Reanalysis and Data Assimilation	10		6	5	5	3.0 %/decade	SSEOB

2.3 IGACO observational requirements on ozone

The IGACO (2004) requirements are platform independent and assume an integrated approach, in the case of ozone using satellites, ozone sondes, *in situ* (aircraft, balloon, surface) and ground-based remote sensing.

Table 3: The IGACO (2004) observational requirements on ozone. In the last column the target and threshold values are separated by a '/'. The delay time between observation and availability of the product: HOURS for operational use in chemical weather forecast, air quality, and oxidation efficiency; DAYS to WEEKS for global distributions, ozone depletion, trend analysis and verification of international agreements; MONTHS for climate research and modelling. LT = lower troposphere; UT = upper troposphere; LS = lower stratosphere; USM = upper stratosphere, mesosphere; TOC = total ozone column; TrOC = tropospheric ozone column.

Horizontal resolution (km)	LT UT LS USM TOC TrOC	<5 / 50 10 / 100 50 / 100 50 / 200 10 / 50 10 / 50
Vertical resolution (km)	LT UT LS USM	2 / 3 2 / 4 2 / 4 2 / 4
Temporal resolution (hr)	LT UT LS USM TOC TrOC	2 2 6-12 24 12 2
Precision (random error (%)	LT UT LS USM TOC TrOC	1 / 5 1 / 10 2 / 20 2 / 4 1 / 5 1 / 5
Trueness (total error) (%)	LT UT LS USM TOC TrOC	2 / 10 2 / 20 2 / 20 5 / 30 2 / 10 2 / 10
Delay	All	HOURS / DAYS to WEEKS

2.4 Across-ECV requirements and international climate modelling

Combined use of different ECVs, including ozone, in climate model evaluations might have additional value and provide new insights on chemical and physical processes in the model. Climate process validations, such as pioneered by the CCMval community for climate-chemistry interactions, are likely to be expanded to the integrated climate system in the next years, and will lead to more sophisticated process-based Earth-System validation exercises.

The ozone ECV products are integral part of these exercises, e.g. related to changes in transport regimes in troposphere and stratosphere, and stratosphere-troposphere dynamical couplings as well as chemistry-climate interactions. Process validation in an Earth-System context would be enhanced by the choice of one or more golden years across the different ECV projects. For example, taken from the perspective of the ozone (profile) observations the year 2008 has been used as golden year in Phase-1 (2010-2013) of the *Ozone_cc*i project.

The stratospheric ozone layer still is and has been an important research topic for the last 40 years, since the discovery of the ozone hole in 1985. In recent years, the focus of scientific investigations is more on ozone-climate connections and the coupling of the troposphere and the stratosphere in a changing climate considering the depletion of the ozone layer in the past and the expected recovery to 1980 levels in future decades. There are several internationally organised activities which are regularly summarising the current status of scientific activities and describing the actual knowledge, in particular pointing out the uncertainties in our current understanding (e.g. WMO, 2022).

The validation of data derived from numerical models is a corner stone of scientific activities. Numerical models are used in combination with observations to understand and explain mean conditions as well as spatial and temporal variability of distinct quantities describing atmospheric conditions and specific features, especially those affecting the ozone layer (SPARC CCMVal, 2010).

Validation of Chemistry-Climate Models (CCMs; see SPARC CCMVal, 2010) has demonstrated that most models are able to simulate spatial structures and temporal behaviour of the ozone layer, but that there are other large uncertainties. For example, measurements prove that tropical lower-stratospheric water vapour amounts decreased by roughly 0.5 parts per million (ppm) around 2000 and remained low through 2009. This followed an apparent but uncertain increase in stratospheric water vapour amounts from 1980-2000.

The mechanisms driving long-term changes in stratospheric water vapour are still not well understood (Dessler et al., 2014). So far, CCMs predict increases of stratospheric water vapour concentrations, but confidence in these predictions is low. Confidence is low since these same models (1) have a poor representation of the seasonal cycle in tropical tropopause temperatures (which control global stratospheric water vapor abundances) and (2) cannot reproduce past changes in stratospheric water vapour abundances. New consolidated water vapour data products in combination with data derived from CCM simulations should help to get a deeper insight in those processes relevant for the short- and long-term variability of the water vapour distribution in the upper troposphere and the stratosphere.

Combined analyses of ozone and water vapour could help the model evaluations. The tropical upper troposphere / lower stratosphere is the atmospheric region where we have the most obvious indication for circulation changes (i.e., increase of tropical upwelling). Long-term ozone measurements provide a link between climate-change, tropical upwelling (as part of the Brewer-Dobson Circulation) and lower tropical ozone.

Tropospheric ozone is a complex result from radiative, dynamical, physical and chemical processes in the atmosphere. The stratosphere is a significant source of tropospheric ozone and dry deposition at the Earth’s surface is an important contributor to ozone removal. Ozone is either chemically destroyed or produced, depending on the chemical regime, principally determined by the presence of nitrogen oxides (NOx) and further modulated by the presence of methane, CO and non-methane hydrocarbons, meteorology, UV radiation, water vapour and clouds. The relative importance of the processes depends on altitude, time and geographic location.

The NO_2 climate data records developed by ESA’s Precursor_cci project (https://climate.esa.int/en/projects/precursors-for-aerosols-and-ozone) will provide important additional information to better understand the chemistry related to tropospheric ozone, both in the background (lightning and convection processes) as well as closer to urban areas (smog formation) and during wildfire events. The large-scale context of tropospheric ozone and its chemistry implies that new insights could emerge when tropospheric NO_2 and tropospheric ozone products are considered in concert both regionally as well as globally.

3 Rationale for ozone products

This section introduces the rationale behind product developments in Ozone_cci. This rationale is basically unchanged with respect to earlier versions of the URD as the arguments remain valid. Some applications of recently available ozone data are described. Gaps regarding missing information (observations) are identified and the additional value of expected data products to be developed is determined. A detailed evaluation of models is a necessary prerequisite for robust assessment studies of the future evolution of the ozone layer. After a short introduction on the role of ozone in the atmosphere and its link with climate, representative CCM applications are briefly introduced (Section 3.2). Available ozone data products used for recent investigations are described in Section 3.3. Section 3.4 provides examples of intercomparison studies carried out for internationally organised evaluation exercises.

3.1 Introduction

Ozone is the most important radiatively active trace gas in the stratosphere. Ozone absorbs the solar radiation between the wavelength range of about 240 to 300 nm. Radiation below 280 nm (UV-C) is extremely dangerous, but is completely absorbed by ozone. Radiation in the wavelength range of 280 to 320 nm, called UV-B radiation, can penetrate through the whole atmosphere, but its intensity is significantly reduced due to ozone absorption (an approximate rule of-thumb is that 1% decrease in stratospheric ozone leads to 2% increase in UV-B radiation reaching the Earth's surface). UV-B has several harmful effects, particularly at damaging DNA. It is a cause of melanoma (and other types of skin cancer) and the formation of eye cataracts. It has also been linked to the damage of some materials, crops, and marine organisms. Ozone in stratosphere is therefore protecting our planet and is sometimes referred to as 'good' ozone.

The absorbed UV radiation by ozone is the main energy source of the stratosphere and establishes much of its temperature structure and dynamics. In the troposphere, the temperature decreases with increasing height, but in the stratosphere the temperature starts to increase due to absorption of solar radiation by ozone. In the troposphere, atmospheric constituents are rapidly mixed, whereas the vertical mixing of gases in the stratosphere is very slow. Ozone affects not only the Earth's radiation budget by absorption of solar UV radiation, but also by the absorption of terrestrial radiation in the infrared atmospheric window near 9.6 µm. As such, ozone acts as a greenhouse gas in the troposphere.

At the Earth's surface, ozone comes into direct contact with life forms and displays its destructive side. It damages forests and crops; destroys nylon, rubber, and other materials; and injures or destroys living tissue. It is a particular threat to people, who exercise outdoors or who already have respiratory problems. When ozone pollution reaches high levels, pollution alerts are issued urging people with respiratory problems to take extra precautions or to remain indoors. Ozone has been linked to tissue decay, the promotion of scar tissue formation, and cell damage by oxidation. It can create more frequent attacks for individuals with asthma, cause eye irritation, chest pain, coughing, nausea, headaches and discomfort. It can worsen heart disease, and bronchitis. Ozone in the troposphere is toxic to human beings and many other living beings that breathe it and therefore it is often referred to as 'bad' ozone.

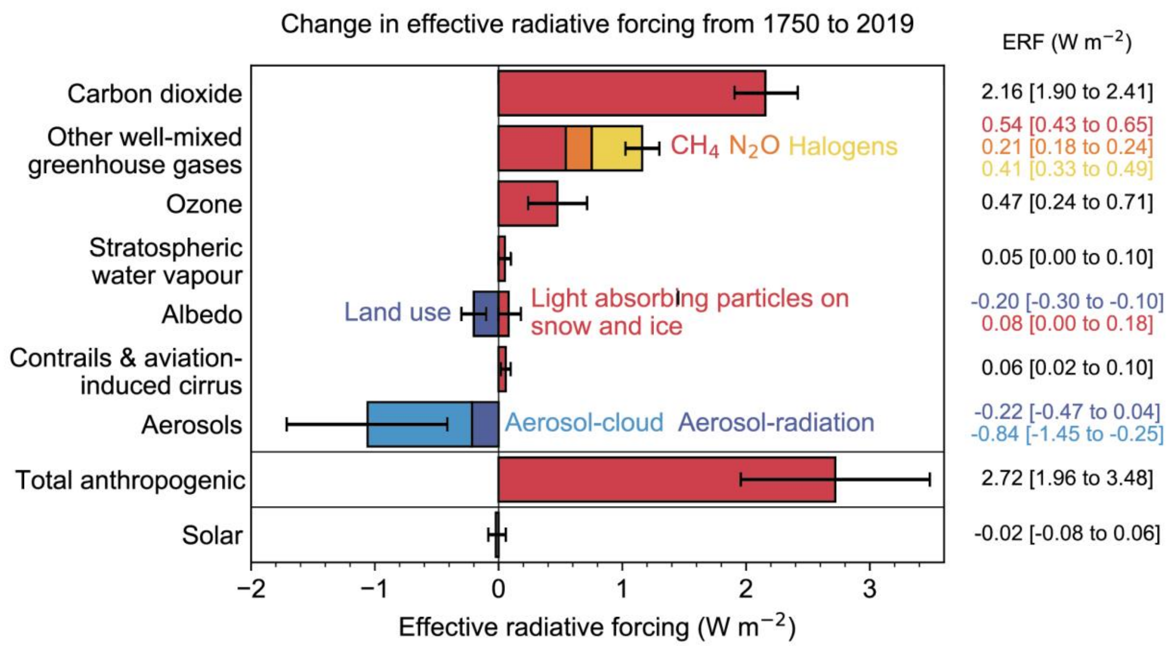

Figure 1: Summary of the principal components of the radiative forcing of climate change. All these radiative forcings result from one or more factors that affect climate and are associated with human activities or natural processes. The values represent the forcings in 2019 relative to the start of the industrial era (about 1750). Human activities cause significant changes in long-lived gases, ozone, water vapour, surface albedo, aerosols and contrails. The only increase in natural forcing of any significance between 1750 and 2019 occurred in solar irradiance. Positive forcings lead to warming of climate and negative forcings lead to a cooling. The thin black line attached to each coloured bar represents the range of uncertainty for the respective value. (Figure 7.6 of IPCC Sixth Assessment Report: Climate Change 2021)

Due to the dual role of ozone, the climate impact of changes in ozone concentrations varies with the altitude at which these ozone changes occur (Figure 1). The major ozone losses that have been observed in the lower stratosphere due to the human-produced chlorine- and bromine-containing gases have a cooling effect on the Earth's surface. On the other hand, the ozone increases that are estimated to have occurred in the troposphere because of air pollution have a warming effect on the Earth's surface, thereby contributing to the greenhouse effect.

The possible combined climate impact of these ozone changes is still not completely understood (e.g. WMO, 2022). Conversely, changes in the climate of the Earth could affect the behaviour of the ozone layer, because ozone is influenced by changes in the meteorological conditions and by changes in the atmospheric composition that could result from climate change. One major issue is that the stratosphere will probably cool in response to climate change, therefore preserving over a longer time period the conditions that promote chlorine-caused ozone depletion in the lower stratosphere, particularly in polar-regions. However higher up in the stratosphere where ozone is primarily constrained by photochemistry, the cooling will reduce the efficiency of ozone loss processes thereby leading to an increase of the ozone concentration and therefore a possible “super-recovery” of the ozone. All these processes still have to be firmly assessed.

3.2 Modelled ozone data

In 2003 the “Stratospheric Processes And their Role in Climate” (SPARC) core project of the World Climate Research Programme (WCRP) initiated the CCM Validation (CCMVal) activity. Since then long-term (decadal) simulations performed with CCMs were internationally coordinated by this activity. CCMVal aimed to improve understanding of CCMs and their underlying general circulation models through process-oriented evaluation, along with discussion meetings and coordinated analyses of science results. In recent years, the model validation activities have been continued in the Chemistry Climate Model Initiative (CCMI) as part of SPARC (now APARC, Atmospheric Processes And their Role in Climate). Coordinated model simulations have been carried out during the preparation phases of the WMO Scientific Assessments of Ozone Depletion. Section 3.4 provides examples of typical results for comparisons between model data and already available data from space-borne observations.

3.3 Observed ozone data

For these evaluation exercises and assessment studies the following ozone data products have been used:

- monthly mean total ozone columns (e.g., derived from TOMS, SBUV/2, OMI, GOME (1+2), and SCIAMACHY);
- data from ozone stations; in parts altitude resolved information from space-borne instruments (e.g. HALOE, MLS, MIPAS).

The above data sets cover different time periods and have been derived from different instruments. For climatological assessments and investigations of long-term changes (i.e., trends) many individual instrument records are too short. Even though TOMS is widely used, the long data set is a result of merging shorter periods observed with different TOMS instruments. Therefore, an obvious problem is that the recent total ozone data sets are mostly not consistently harmonised and do not provide a solid basement for robust analyses of short- and long-term fluctuations. That is why the scientific community falls back upon using different data sets or merged data for those investigations (see Section 3.3), making reliable scientific conclusions difficult. Merged data sets are often based on data assimilation techniques, i.e. techniques build upon numerical model systems which on their part have uncertainties due to specific assumptions (e.g. parameterisations, simplifications, interpolation). The total uncertainty of such data products is often unknown, and the accuracy of given values is mostly undefined.

Moreover, vertically resolved information (ozone profiles) on longer time scales (decades) are rare; so far it is mostly available from single observation wards (e.g. ground based measurements, radiosondes), i.e. global coverage is weak, particularly in the Southern Hemisphere.

In the following, wherever necessary, Level-2 (orbits), Level-3 (gridded), and Level-4 (assimilated) final data products are distinguished.

3.4 Linking modelled and observed ozone data

This section provides illustrations of typical evaluations of ozone data derived from CCM simulations. These show how available data products are used for evaluation purposes to identify strengths and weaknesses of the models. The given examples demonstrate that the evaluation of numerical models will benefit substantially from improved observational data products.

Figure 2 shows a comparison of measurements provided by the satellite instrument MLS (Microwave Limb Sounder, onboard of the Upper Atmosphere Research Satellite, UARS) with results derived from 18 different CCMs (Chapter 2 in SPARC CCMVal, 2010; updates in Dhomse et al., 2018; Keeble et al., 2021). Note that the comparison is limited to values describing the monthly deviations from annual mean values; no information is provided about absolute values. The analysis shows that the annual cycle of ozone at 1 hPa (stratopause region) and 46 hPa (lower stratosphere) is mostly well reproduced by the CCMs, although there are obvious differences in detail.

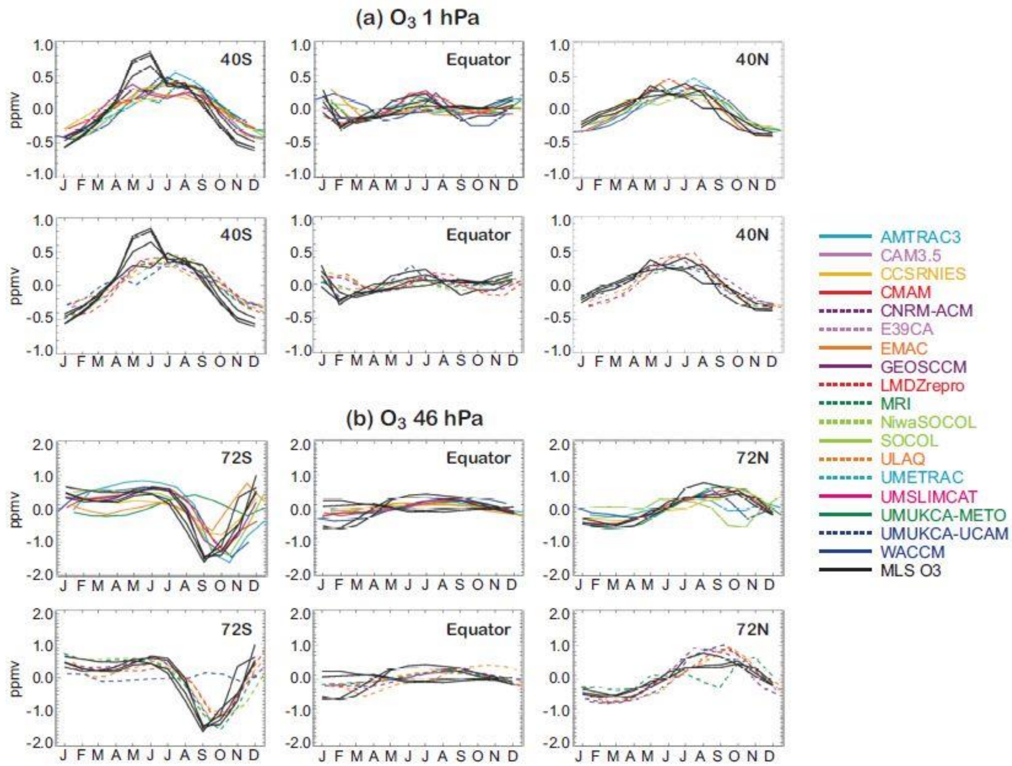

Figure 2: Anomalies of monthly mean ozone mixing ratios (in ppmv) at 1 hPa throughout the year, 40°S (left), Equator (middle) and 40°N (right) from several years of MLS observations (black lines) and for the CCMVal-2 CCMs (monthly zonal-mean ozone in the early 2000s from selected years; colour lines). MLS data are averaged for a 6° latitude band centred on the selected latitudes. (b) Same as (a) but at 46 hPa, 72°S (left), Equator (middle), and 72°N (right). (Figure 8-2 from SPARC CCMVal, 2010.)

Figure 3 shows comparisons of vertically resolved information derived from HALOE (Halogen Occultation Experiment, also onboard of UARS) with CCM data. The comparison is based on monthly mean values (due to the sparse global coverage during a single month); obviously, the availability of ozone data in the Polar Regions is small. Beneficial is the provision of an uncertainty range in HALOE data, here given as a standard deviation.

Figure 4 illustrates the long-term evolution of total ozone values in a specific latitudinal region (in this case the southern polar hemisphere). Observations are included in the three sub-figures, representing the “reality” for the recent past. In this particular case, observations (indicated by “OBS”) are a merged data set compiled from different sources, including ground-based observations, especially used in the period before 1979. Here the observations are given without any indication of a range of uncertainty.

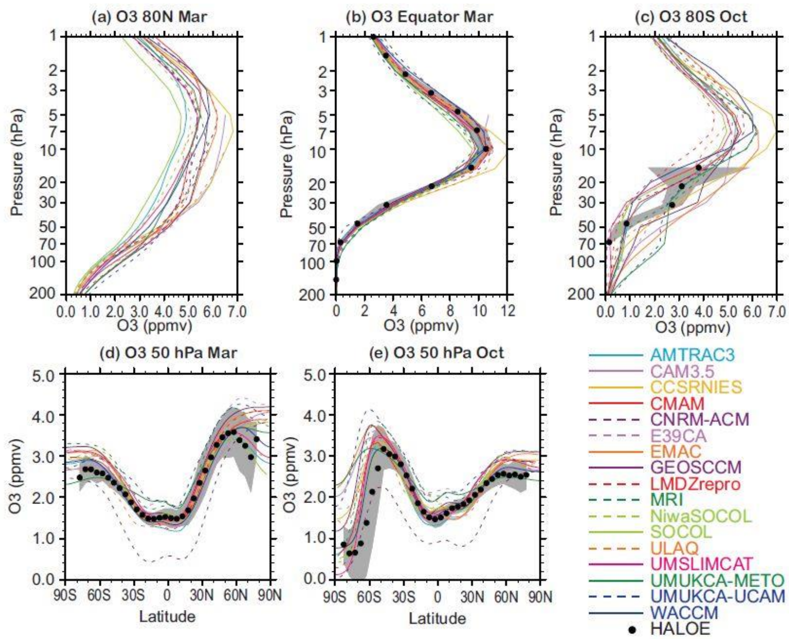

Figure 3: Climatological zonal mean ozone mixing ratios from CCMs and HALOE (in ppmv). Vertical profiles at (a) 80°N in March, (b) Equator in March, and (c) 80°S in October. Latitudinal profiles at 50 hPa in (d) March and (e) October. The grey area shows HALOE ±1 standard deviation (s) about the climatological zonal mean. (Figure 8-3 from SPARC CCMVal, 2010.)

Figure 5 gives an example of a comparison of climatological mean CCM data to a (merged) multi-sensor satellite data record. This prototype data record combines total ozone measurements by GOME (ERS-2), SCIAMACHY (Envisat) and GOME-2 (MetOp-A) yielding a continuous time series starting in June 1995 (Loyola et al., 2009).

Statistical analyses, e.g., to investigate the internal variability of the atmospheric (model) system (as presented in Figure 6) requires long-term time series. This is the basis for the detection of statistically significant changes. A detailed knowledge of such parameters (in observations as well as in model results) is a necessary prerequisite to distinguish between regular fluctuations of the atmospheric system and abnormal changes. At least such a comparison provides another possibility to check the quality of the atmospheric model.

Figure 7 illustrates another conventional confrontation of measured and modelled data. In this case, the aim is to demonstrate that the model is able to reproduce both short- and long-term fluctuations adequately. Moreover, it is used to demonstrate the reliability of the model, in particular with regard to the assessment of the future evolution of the ozone layer.

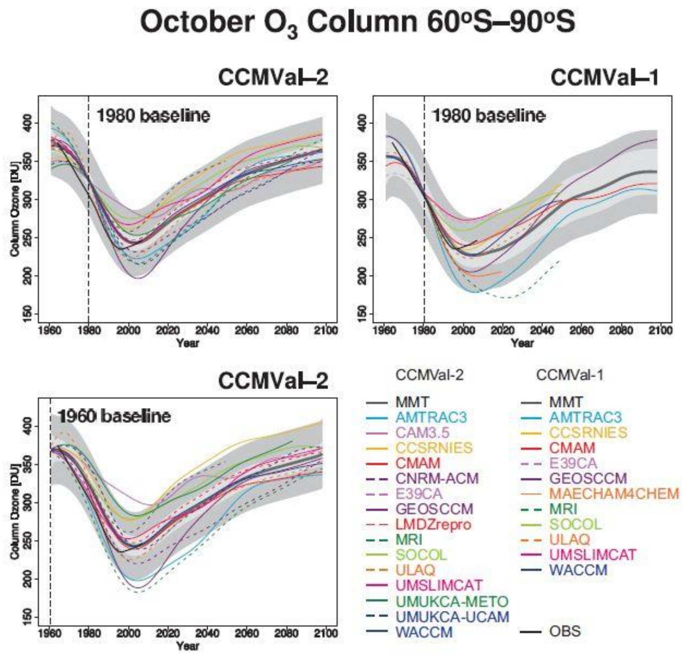

Figure 4: 1980 baseline-adjusted multi-model trend (MMT) estimates of annually averaged total ozone for the latitude range 60°S-90°S for the month of October (heavy dark grey line) with 95% confidence and 95% prediction intervals appearing as light- and dark-grey shaded regions about the trend (upper panels). The baseline-adjusted individual model trend estimates, and unadjusted lowness fit to the observations are additionally plotted. CCMVal-2 results appear on the left and CCMVal-1 results appear on the right. The lower panel shows the same analysis of CCMVal-2 data but for a baseline adjustment employing a 1960 reference date. (Figure 9-12; SPARC CCMVal, 2010)

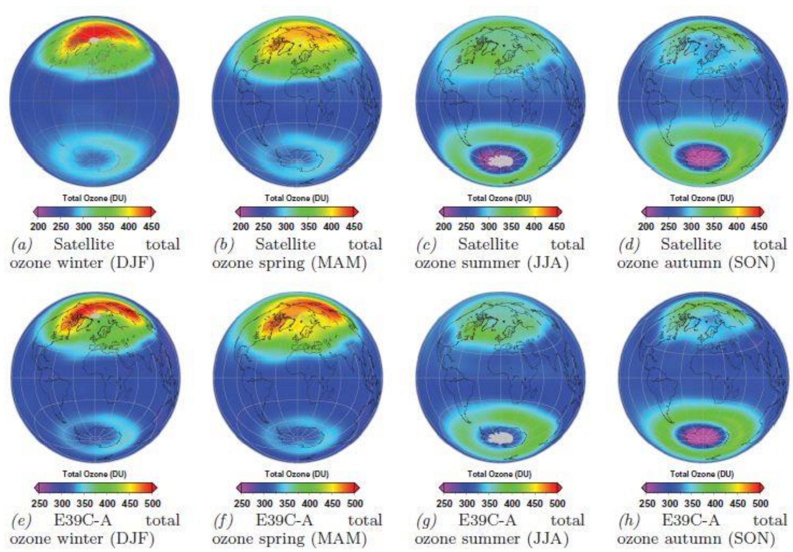

Figure 5: Seasonal mean values of total ozone (June 1995 to May 2008, in Dobson Units, DU) from a merged satellite record (GOME, SCIAMACHY, GOME-2; top) and the CCM E39C-A simulation (bottom) (Figure 9; Loyola et al., 2009).

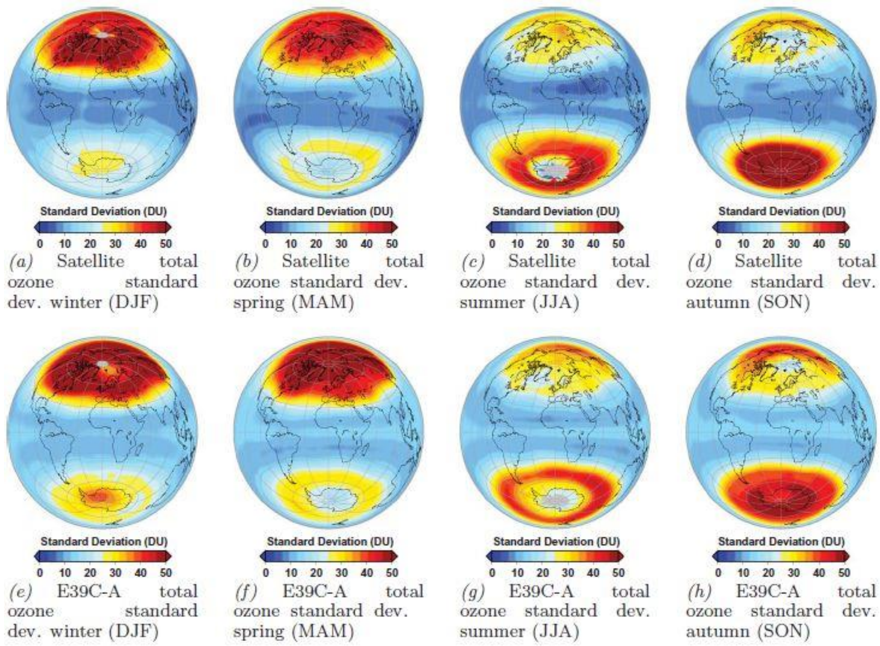

Figure 6: Seasonal mean values of total ozone standard deviations (June 1995 to May 2008, units: DU) from satellite instruments (top) and the E39C-A simulation (bottom) (Figure 7; Loyola et al., 2009).

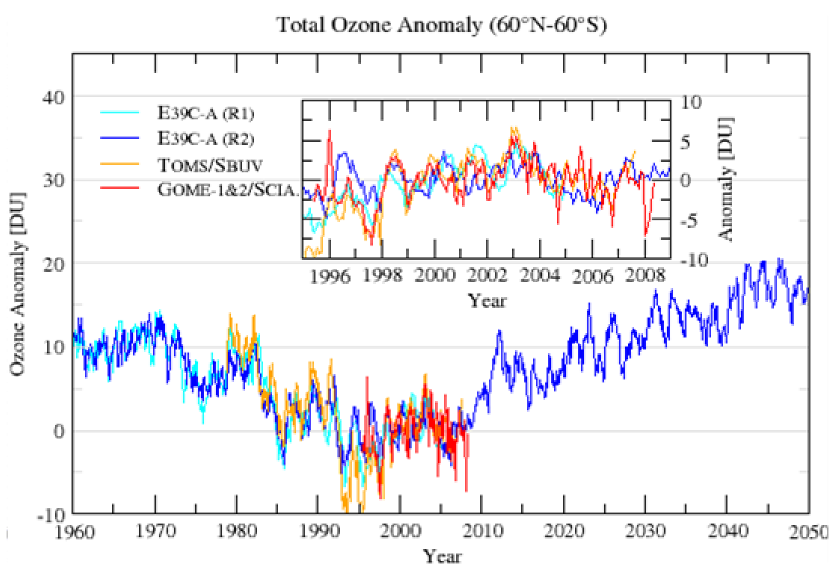

Figure 7: Total ozone anomalies over 60°N to 60°S. The mean annual cycle for 1995 to 2004 is subtracted from satellite measurements (orange and red) and two E39C-A model simulations R1 from 1960 to 2004 (cyan) and R2 from 1960 to 2050 (blue). The inset shows a close-up for years where satellite measurements are available (Update of Figure 9; Loyola et al., 2009).

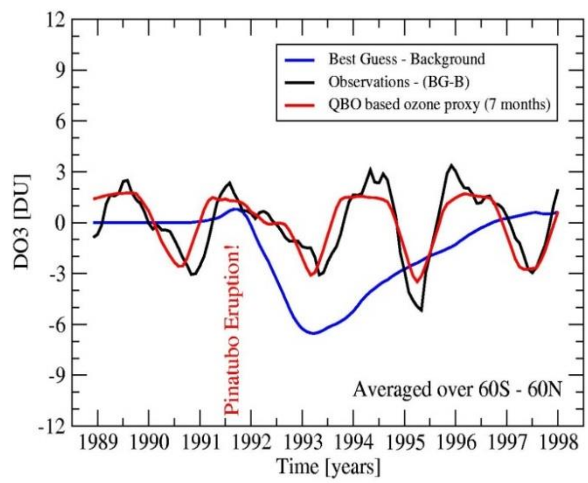

Figure 8: Time series of global ozone anomalies. Blue: ozone change due to volcanic aerosol; Black: residual ozone change; Red: a QBO based ozone proxy. Note the good agreement between the black and red line.

Models in conjunction with high quality observations can be used to attribute ozone changes. Telford et al. (2009) used a CCM to attribute the ozone loss due to the eruption of Mt Pinatubo in 1991. The blue line in Figure 8 shows the quasi-global ozone loss modelled in their nudged CCM. Subtracting the modelled ozone loss from the observed ozone produces a residual "dynamical" ozone change that correlates very well with the QBO. Such an exercise provides two valuable results: A consistency check of the CCM and a quantification of an attributable signal.

These examples demonstrate how evaluation of model results (here derived from CCMs) has been typically done in recent years. The main deficiencies of available ozone data sets derived from satellite sensors for a complete evaluation of climate models and CCMs are the following:

(1) Individual measurements for the same time period from different satellite instruments often show significant absolute differences; short- and long-term fluctuations show different behaviour including varying amplitudes of anomalies;

(2) consistent time series are too short to perform reliable climatological mean values and robust statistical analyses, particularly in the Northern Hemisphere;

(3) consistent ozone data series are not long enough to investigate long-term changes (i.e. trends);

(4) consistent vertically resolved, global information of atmospheric ozone content is not available for longer periods (i.e. several years) to investigate long-term variability and trends at different altitudes separately;

(5) detailed estimates of total errors (i.e. range of uncertainty including instrument drift etc.) of data products derived from satellite measurements are rarely available.

The end data products which are created in the Ozone_cci project, i.e. merged regridded, multi-sensor data sets covering long-term (multi-year) periods, represent a significant additional value to recently available data products because they will obviously reduce the abovementioned inadequacies.

4 Product requirements and traceability

4.1 Introduction

ECV data sets produced within the Ozone_cci project fall into two categories, a column integrated product (total ozone, including separate tropospheric and stratospheric ozone columns) and vertically resolved products (from limb and nadir sounders). Product requirements reflect the nature of the products. Each data value is required to have an error bar. In the case of total ozone (expressed in DU, x) the error will be given as a delta total ozone value in DU (δx), such that x±δx represents at least a 95% confidence interval. In the case of limb ozone profiles two error bars are required, one representing an altitude range the other representing a volume mixing ratio range and both representing at least a 95% confidence interval. Figure 9 illustrates this requirement. From a climate modelling perspective, it would be acceptable to translate the height error into an additional mixing ratio error. Other applications, like data assimilation, might prefer a distinct reporting of errors.

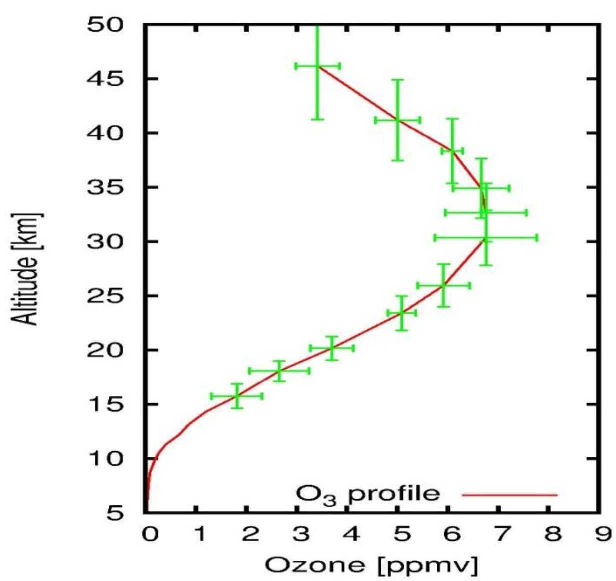

Figure 9: Sketch illustrating an ozone profile and the reporting of errors.

All ozone ECV products should cover continuously extended time periods, preferably decadal and beyond. We realise that the typical lifetime of a satellite mission is sometimes shorter; therefore, data sets have to be merged into a FCDR. Records (user-friendly data sets) need to be built from Level-2 data, and can be advanced into Level-3 and Level-4 data. For example, a Level-2 data record relevant for data assimilation applications can be organised by satellite orbit. A Level-3 data record has added value by aggregating Level-2 data on a regular grid. Furthermore, different instruments can be merged into one Level-3 data record. A product using a numerical model (data assimilation) to generate a value added data from any lower level set is called Level-4. The requirement tables in this section distinguish between research topics and identify targets achievable within the Ozone_cci project. Targets that should be aspired to in future missions to improve our research capability are identified as well.

4.2 Total ozone data product

Traditionally, total ozone has been used as monthly mean data with an extensive global coverage (60°S to 60°N, see WMO/UNEP Scientific Assessment of Ozone Depletion: 2022). To understand better the seasonal evolution of ozone, the time for global coverage should be no longer than 3 days. A good temporal coverage allows the assessment of climatologically important blocking events and regional ozone changes. Regional assessments will not only require a good temporal resolution, but a good spatial resolution as well (on the order of 100 km). Many numerical models of the atmosphere have grids that converge towards the poles – effectively their spatial resolution becomes better at higher latitudes. Therefore, it would be useful if resolutions below 100 km could be achieved. For the detection of ozone trends (rate of change per decade) the stability should be significantly smaller than the trend (e.g. half). The relevance of this requirement depends of course on the length of the records available. Ancillary requirements include cloud information per pixel (including cloud fraction, cloud height, cloud albedo) and surface information per pixel (surface albedo).

Requirements are given on Level-2 which is the required level for data assimilation applications. Aggregated multi-sensor Level-3 products should retain these Level-2 requirements as much as possible. At least, Level-3 products should not be homogenized/degraded to the instrument with the smallest uncertainty over the targeted time period.

The required precision is included in the error budget expressed as (total) uncertainty and would be the same as for the tabulated uncertainty under the (unrealistic) assumption that all biases in the products could be fully characterized.

Table 4: Requirements for total ozone column fundamental climate data records (FCDRs). The ozone total column requirements are for ozone products in terms of Dobson Units (i.e. the vertically integrated number of ozone molecules per unit area; 1 DU = 2.69 x 10^{16} molec. cm^{-2}). Achievable and future target requirements are given, separated by a '–', the first number is the future target.

		Geographical Zone		
Quantity	**Driving Research topic**	**Tropics**	**Mid-latitudes**	**Polar region**
Global horizontal resolution	Evolution of the ozone layer (radiative forcing); Seasonal cycle and interannual variability; Short-term variability* (Exchange of air masses, streamers, regime studies)	20 – 100 km	20 – 50/100 km	20 – 50/100 km
Observation frequency	Evolution of the ozone layer (radiative forcing); Seasonal cycle and interannual variability; short-term variability*	Daily – weekly	Daily – weekly	Daily – weekly
Time period	Evolution of the ozone layer (radiative forcing)	(1980 -)	(1980 -)	(1980 -)
Uncertainty	Evolution of the ozone layer (radiative forcing)	2% (7 DU)	2% (7 DU)	2% (7 DU)
Uncertainty	Seasonal cycle and interannual variability; Short-term variability*	3% (10 DU)	3% (10 DU)	3% (10 DU)
Stability (after corrections)	Evolution of the ozone layer (trend detection; radiative forcing)	1 – 3% / decade	1 – 3% / decade	1 – 3% / decade

* Short-term variability includes: Exchange of air masses, streamers, regime studies.

Table 5: Data requirements for total ozone column fundamental climate data records (FCDRs).

Data feature	Requirement
Data format	netCDF
Data conventions	CF
Data units	Total column (in DU; number of molecules per area or equivalent)
Error	Total area
Error characteristics (optional)	Total uncertainty and its subdivision per pixel into: - contribution measurement noise; - contribution of A Priori uncertainties; - contribution of estimated spectroscopic uncertainty
Averaging kernels	Yes, for Level-2
Full covariance matrix included ?	No
A priori data	Yes, per pixel
Quality flag	1: high quality data 2: contaminated data 3: missing value
Visualisations	Basic browsable archive visualisation (daily global maps; local/latitudinal time series of monthly means)

4.3 Ozone profile and tropospheric ozone data products from nadir-viewing instruments

Ozone profile data requirements are product and application specific. Current data requirements should reflect the actual resolutions of numerical models used at the moment. For example, chemistry-climate models (CCMs) have typical horizontal resolutions in the order of 200 km at the equator and vertical resolutions of ~1 km in the upper troposphere and lower stratosphere. CCMs resolve explicitly the troposphere and the stratosphere. For the nadir-viewing instruments, the intrinsic coarser vertical resolution (~6 km) is acceptable. Nadir ozone profiles observations typically have a very good horizontal coverage. Partial columns observations therefore provide an alternative to high-resolution vertical profiles. It is useful if the (partial) columns are assimilated into a Level-4 product which can provide enhanced vertical resolution relative to the nadir observations. The vertical resolution in the upper troposphere and lower stratosphere (UTLS) region is of particular importance for the Earth climate system including surface climate. The temporal resolution should be in agreement with the total ozone requirements – this will make consistency checks and attribution studies straightforward. The targeted time period for the nadir ozone profiles would start from 1996 onward. Ancillary requirements include cloud information per pixel (including cloud fraction, cloud height, cloud albedo) and surface information per pixel (surface albedo).

As part of the *Operoz* study (ESA, 2015) long-term monitoring ozone profile requirements have been re-evaluated and compared to the user requirements during Phase 1 (2010-2013) of the *Ozone_cci* project. Important elements in this re-evaluation that have been taken on board in this URD include:

- Definition of Middle Atmosphere as the atmosphere above 30 km.
- Definition of Lower Stratosphere as the layer between the tropopause and 30 km.
- The tropopause is defined by the (pressure) altitude using the WMO temperature criterium (< 2 K/km) or the (pressure) altitude above which the ozone mixing ratio continues to exceed 150 ppbv.
- A 8% target for daily 6 km resolution nadir ozone profile information up to the lower stratosphere and an achievable requirement of 16% on a weekly basis.
- A data unit requirement for ozone observations in volume mixing ratio and optionally also in partial column and/or provided with a co-located temperature profile.

Requirements are given on Level-2 which is the required level for data assimilation applications. Aggregated multi-sensor Level-3 products should retain these Level-2 requirements as much as possible. At least, Level-3 products should not be homogenized/degraded to the instrument with the smallest uncertainty over the targeted time period. The required precision is included in the error budget expressed as (total) uncertainty and would be the same as for the tabulated uncertainty under the (unrealistic) assumption that all biases in the products could be fully characterized.

Table 6: Product requirements for nadir-based ozone profile fundamental climate data records (FCDRs). The ozone profile requirements are for ozone products in terms of (partial-column mean) mixing ratios. The tropospheric altitude domain extends from the surface to the tropopause defined by an ozone concentration of 150 ppbv; the UT/LS extends from about 5 to 30 km, and the middle atmosphere extends from about 30 to 60 km altitude. The required coverage is global. Achievable and future target requirements are given, separated by a '–'. The first number is the future target.

		Height range		
Quantity	**Driving Research topic**	**Troposphere**	**UT/LS**	**Middle Atmosphere**
Horizontal resolution	Regional differences in evolution of the ozone layer and tropospheric ozone burden (radiative forcing); Seasonal cycle and interannual variability; Short-term variability	20 – 200 km	20 – 200 km	200 – 400 km
Vertical resolution	Height dependence of evolution of the ozone layer and the tropospheric ozone burden (radiative forcing); Seasonal cycle and interannual variability; Short-term variability	6 km – tropospheric column	6 km – partial column	6 km – partial column
Observation frequency	Evolution of the ozone layer and the tropospheric ozone burden (radiative forcing); Seasonal cycle and interannual variability; Short-term variability	Daily – weekly	Daily – weekly	Daily – weekly
Time period	Evolution of the ozone layer and tropospheric ozone burden (radiative forcing)	(1980 -)	(1980 -)	(1980 -)
Uncertainty	Evolution of the ozone layer and tropospheric ozone burden (radiative forcing)	8%	8%	8%
Uncertainty	Seasonal cycle and interannual variability; Short-term variability	16%	16% (< 20 km) 8% (> 20 km)	8%
Stability	Evolution of the ozone layer and tropospheric ozone burden (radiative forcing); trends	1 – 3% / decade	1 – 3% / decade	1 – 3% / decade

Table 7: Data requirements for nadir-based ozone profile fundamental climate data records (FCDRs)

Data feature	Requirement
Data format	netCDF
Data conventions	CF
Data units	Ozone mixing ratio (optional: also in partial ozone column and/or with co-located temperature profile)
Error characteristics	Total uncertainty and its subdivision per pixel and per layer into: - contribution measurement noise; - contribution smoothing error - contribution of A Priori uncertainties;
Number of layers	To be chosen for optimal accuracy (not too few for information content, not too many by degrading the accuracy per layer)
Averaging kernels included ?	Yes, per pixel
Full covariance matrix included ?	Yes, per pixel
A priori data included ?	Yes, per pixel
Flags	Quality per pixel (good, bad, uncertain); Pixel type; Snow/ice; Sun glint; Solar Eclipse; South-Atlantic Anomaly
Visualisations	Basic browsable archive visualisation (profile cross section per orbit; monthly maps at standard pressure levels; local/latitudinal time series of monthly means at standard pressure levels)

4.4 Ozone profile data product from limb-viewing instruments

Data requirements are product and application specific. Current data requirements should reflect the actual resolutions of numerical models used at the moment. For example, chemistry-climate models (CCMs) have typical horizontal resolutions in the order of 200 km at the equator and vertical resolutions of ~1 km in the upper troposphere and lower stratosphere. For practical purposes of monitoring a coarser vertical resolution is acceptable (~3 km), but a higher vertical resolution (<1 km) should be aspired to. The time resolution should be in agreement with the total ozone requirements – this will make consistency checks and attribution studies straightforward. The minimum targeted time period for the limb ozone profiles covers the period starting from 2003 onward. For climate research long term records are needed. Many short-term processes as well as seasonality and inter-annual variability in ozone in climate models can already be validated with a couple of years. Ancillary requirements include cloud information per profile including cloud fraction, cloud height and the temperature profile.

As part of the *Operoz* study (ESA, 2015) long-term monitoring ozone profile requirements have been re-evaluated and compared to the user requirements during Phase-1 (2010-2013) of the *Ozone_cci* project. The *Operoz* study focused on the ozone profile user requirements at high vertical resolution. Important elements in this re-evaluation that have been taken on board in this document include:

- Definition of middle atmosphere as the atmosphere above 30 km.
- Definition of lower stratosphere as the layer between the tropopause and 30 km.
- The tropopause is defined by the (pressure) altitude using the WMO temperature criterium (< 2 K/km) or the (pressure) altitude above which the ozone mixing ratio continues to exceed 150 ppbv.
- A 8% (> 20 km) and 16% (< 20 km) target for daily 1 km resolution ozone profile information per 100 km in the lower stratosphere and an achievable requirement of 2 km resolution weekly profiles per 200 km.
- A 8% target for daily 2 km resolution ozone profile information per 200 km in the middle atmosphere and an achievable requirement of 4 km resolution weekly profiles per 400 km.
- A data unit requirement for ozone observations in volume mixing ratio and optionally also in partial column and/or provided with a co-located temperature profile.

Table 8: Product requirements for limb-based ozone profile fundamental climate data records (FCDRs). The ozone profile requirements are for ozone products in terms of (partial-column mean) mixing ratios. The lower stratosphere (LS) extends from the tropopause (defined as ozone > 150 ppbv) to about 30 km, and the middle atmosphere extends from about 30 to 60 km altitude. The required coverage is global. Achievable and future target requirements are given, separated by a '–'. The first number is the future target.

		Height Range	
Quantity	**Driving Research topic**	**Lower Stratosphere**	**Middle Atmosphere**
Horizontal resolution	Regional differences in the evolution of the ozone layer (radiative forcing); Seasonal cycle and interannual variability; Short-term variability	100 – 200 km	200 – 400 km
Vertical resolution	Height dependence of evolution of the ozone layer (radiative forcing); Seasonal cycle and interannual variability; Short-term variability	1 – 2 km	2 – 4 km
Observation frequency	Seasonal cycle and interannual variability; short-term variability	Daily – weekly	Daily – weekly
Time period	Evolution of the ozone layer (radiative forcing)	(1980-)	(1980-)
Uncertainty in height attribution	Evolution of the ozone layer(radiative forcing), Seasonal cycle and interannual variability; Short-term variability	±500 m	±500 m
Uncertainty for mixing ratio	Evolution of the ozone layer (radiative forcing)	8%	8%
Uncertainty for mixing ratio	Seasonal cycle and interannual variability; Short-term variability	16% (< 20 km) 8% (> 20 km)	8%
Stability	Evolution of the ozone layer (radiative forcing); trends	1 – 3% / decade	1 – 3% / decade

Requirements are given on Level-2 which is the required level for data assimilation applications. Aggregated multi-sensor Level-3 products should retain these Level-2 requirements as much as possible. At least, Level-3 products should not be homogenized/degraded to the instrument with the lowest accuracy over the targeted time period. The required precision is included in the error budget expressed as (total) uncertainty and would be the same as for the tabulated uncertainty under the (unrealistic) assumption that all biases in the products could be fully characterized.

Table 9: Data requirements for limb-based ozone profile fundamental climate data records (FCDRs).

Data feature	Requirement
Data format	NetCDF
Data conventions	CF
Data units	Ozone mixing ratio (optional: also in partial ozone column and/or with co-located temperature profile)
Error characteristics	Total uncertainty and its subdivision per profile per layer into: - contribution measurement noise; - contribution horizontal smoothing error - contribution pointing accuracy - contribution of A Priori uncertainties;
Averaging kernels included ?	Yes, per profile
Full covariance matrix included ?	Yes, per profile
A priori data included ?	Yes, per profile
Flags	Quality per profile per layer (good, bad, uncertain); Cloud contamination; Solar Eclipse; South-Atlantic anomaly
Visualisations	Basic browsable archive visualisation (profile cross section per orbit; monthly maps at standard pressure levels; local/latitudinal time series of monthly means at standard pressure levels)

4.5 Tropospheric ozone data products

Three complementary techniques are employed to derive tropospheric ozone data products: Convective Cloud Differential (CCD), Limb-Nadir Matching (LNM) and Optimal Estimation (OE) of nadir ozone profiling. Requirements on the troposphere based on the ozone profile retrieval from nadir products are already found in Section 4.3 and repeated in the table below. The Convective Cloud Differential (CCD) technique combines total ozone and cloud information from a nadir sensor to compute a tropospheric column of ozone over clear-sky scenes. The CCD technique is inherently limited to the tropical belt (20°S-20°N) and contains a partial column between surface and 200 hPa (~12 km) or 270 hPa (~10 km). In the tropics, these columns cover at most a bit more than half the troposphere. The CCD technique relies on the availability of total ozone column and cloud data. Data from seven UV-visible nadir sensors can be considered, starting with GOME in 1995 and continuing to this day with several sensors based on an evolved GOME instrument design.

Table 10: Product requirements for the tropospheric ozone profile fundamental climate data records (FCDRs). The ozone profile requirements are for ozone products in terms of (partial-column mean) mixing ratios. The tropospheric altitude domain extends from the surface to the tropopause defined by an ozone concentration of 150 ppbv.. The required coverage is global though not for the CCD technique-based tropospheric ozone products. Achievable and future target requirements are given, separated by a '–'. The first number is the future target.

Quantity	Driving Research topic	Height range		
		Tropospheric column	Upper troposphere	Lower Troposphere
Horizontal resolution	Regional differences in tropospheric ozone burden (radiative forcing); Seasonal cycle and interannual variability; Short-term variability	20 – 200 km	20 – 200 km	< 20 km
Vertical resolution	Height dependence of evolution of tropospheric ozone burden (radiative forcing); Seasonal cycle and interannual variability; Short-term variability	n/a	< 6 km	< 6 km
Observation frequency	Evolution of tropospheric ozone burden (radiative forcing); Seasonal cycle and interannual variability; Short-term variability	Daily – weekly	Daily – weekly	Hourly – weekly
Time period	Evolution of tropospheric ozone burden (radiative forcing)	(1980 -)	(1980 -)	(1980 -)
Uncertainty	Evolution of tropospheric ozone burden (radiative forcing)	8%	8%	8%
Uncertainty	Seasonal cycle and interannual variability; Short-term variability	16%	16%	8%
Stability	Evolution of tropospheric ozone burden (radiative forcing); trends	1 – 3% / decade	1 – 3% / decade	1 – 3% / decade

Table 11: Data requirements for tropospheric ozone profile fundamental climate data records (FCDRs)

Data feature	Requirement
Data format	netCDF
Data conventions	CF
Data units	Ozone mixing ratio (optional: also in partial ozone column and/or with co-located temperature profile)
Error characteristics	Total uncertainty and its subdivision per pixel and per layer into: - contribution measurement noise; - contribution smoothing error - contribution of A Priori uncertainties;
Number of layers	To be chosen for optimal accuracy (not too few for information content, not too many by degrading the accuracy per layer)
Averaging kernels included ?	Yes, per pixel
Full covariance matrix included ?	Yes, per pixel
A priori data included ?	Yes, per pixel
Flags	Quality per pixel (good, bad, uncertain); Pixel type; Snow/ice; Sun glint; Solar Eclipse; South-Atlantic Anomaly
Visualisations	Basic browsable archive visualisation (profile cross section per orbit; monthly maps at standard pressure levels; local/latitudinal time series of monthly means at standard pressure levels)

4.6 Recommendations on Level-1 data product from climate user perspective

The quality of Level-1 is essential, but the relationship with Level-2 and Level-3 data products is primarily up to the retrieval specialists. Therefore, there are no requirements on Level-1 data products from a climate user perspective.

5 References

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