Ozone_cci+

User Requirements Document (URD)

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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.
5	0	16/06/2025	Add section of requirements for an UTLS ozone product by the community and requirements for a geostationary satellite. Update CMUG table. Update figure 1 to show double role of ozone again. Update of figures in section 3 to more recent applications for satellite products used to evalute CCMs. Some minor revisions. Section added about requirements for a geostationary satellite tropospheric ozone product.
5	1	28/11/2025	Harmonised UTLS definition, removed IGACO and cross-ECV requirements sections.

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 3 of this project (2025-2026) the development of existing Essential Climate Variables (ECVs) is continued. Furthermore, new products will be developed: limb profile data tailored to studies of the Upper Troposphere Lower Stratosphere (UTLS) and a prototype nadir profile product from geostationary sounders. This URD v5.1 is similar in content to earlier versions of the URD and mainly expands on the UTLS user needs and information on the requirements for geostationary satellite products. 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 product 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 Essential Climate Variable (ECV) 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; GCOS-107; GCOS-138; GCOS-143; GCOS-244 and GCOS-245), the CMUG, 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 updated GCOS requirements.

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. This version 5.1 (October 2025) introduces requirements for UTLS limb profile products and geostationary tropospheric column products.

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, for each 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. Two new products are added in this phase and introduced in Chapter 4 as well: an Upper Troposphere/Lower Stratosphere (UTLS) ozone profile product referenced to the tropopause height based on limb-viewed satellite products, and a tropospheric ozone product based on geostationary satellite products.

1.3 *Applicable documents*

CMUG, 2024: Climate Community Requirements, Deliverable 1.1, Climate Modelling User Group, version 4, May 2024

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-use 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's 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 are 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; entry 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 h / 30 d	minutes / hours / days
Timeliness	60 min / 24 h / 30 d	minutes / hours / days
Measurement uncertainty	1 / 2 / 3	%
Stability	1 / 2 / 3	% dec^{-1}

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 h / 30 d	minutes / hours / days
Timeliness	6 h / 24 h / 30 d	minutes / hours / days
Measurement uncertainty	1 / 3 / 5	%
Stability	1 / 2 / 3	% dec^{-1}

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 h / 30 d	minutes / hours / days
Timeliness	60 min / 24 h / 30 d	minutes / hours / days
Measurement uncertainty	5 / 10 / 15	%
Stability	1 / 2 / 3	% dec^{-1}

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 h / 30 d	minutes / hours / days
Timeliness	60 min / 24 h / 30 d	minutes / hours / days
Measurement uncertainty	2 / 5 / 10	%
Stability	1 / 2 / 3	% dec^{-1}

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 h / 24 h / 30 d	hours / days
Timeliness	6 h / 24 h / 30 d	hours / days
Measurement uncertainty	2 / 5 / 10	%
Stability	1 / 2 / 3	% dec^{-1}

Mole fraction MUS (no. 1013)	G / B / T	Unit
Horizontal resolution	20 / 100 / 500	km
Vertical resolution	1 / 3 / 10	km

Observing cycle	6 h / 24 h / 30 d	hours / days
Timeliness	4 h / 24 h / 30 d	hours / days
Measurement uncertainty	5 / 10 / 15	%
Stability	1 / 2 / 3	% dec^{-1}

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, D1.1, version 4, May 2024, Table 19). The error type is a single sensor uncertainty estimate for every observation (SSEOB). The requirements are based on a CMUG Survey.

Parameter	Application	Horizontal resolution (km)	Vertical Resolution (km)	Observing Cycle (h)	Precision (%)	Accuracy (%)	Stability (% dec^{-1})
Ozone profile							
Higher stratosphere & mesosphere (HS & M)	Model Development and Evaluation	100	3	24	5	10	2
	Reanalysis and Data Assimilation	50	1	6	5	10	2
Lower stratosphere (LS)	Model Development and Evaluation	50	2	24	3	6	2
	Reanalysis and Data Assimilation	20	1	6	3	6	2
Higher troposphere (HT)	Model Development and Evaluation	20	2	24	3	8	2

Parameter	Application	Horizontal resolution (km)	Vertical Resolution (km)	Observing Cycle (h)	Precision (%)	Accuracy (%)	Stability (% dec^{-1})
	Reanalysis and Data Assimilation	20	1	6	3	6	2
Lower troposphere (LT)	Model Development and Evaluation	20	2	24	6	10	2
	Reanalysis and Data Assimilation	20	1	4	5	10	2
Ozone column							
Troposphere column	Model Development and Evaluation	20		24	6	15	2
	Reanalysis and Data Assimilation	20		4	5	10	2
Total column	Model Development and Evaluation	20		24	2	4	1
	Reanalysis and Data Assimilation	20		6	3	5	1

2.3 *UTLS research communities*

The Upper Troposphere Lower Stratosphere (UTLS) is a critical region of the atmosphere that plays a vital role in shaping our climate. Located between approximately 6 km and 20 km altitude (Operoz study; ESA, 2015), the UTLS acts as a bridge between the troposphere and the stratosphere, exchanging heat and moisture with both lower and upper atmospheric layers. Investigating the UTLS is essential for improving our understanding of climate processes, as its radiative feedback is identified as one of the important drivers for surface climate. However, this region remains one of the most challenging areas to study due to its extreme conditions, such as high altitudes, and processes on several different scales, from turbulence to global circulations, which make data collection and analysis extremely difficult. As a result, there are still significant uncertainties in our knowledge of the UTLS and how it will change in the future.

Table 4: The UTLS user community requirements on ozone. The requirements are based on a survey sent to members of the UTLS scientific communities, the OCTAV-UTLS and TPChange communities. Uncertainty and Stability refer to ozone partial columns per vertical level.

	Unit	Min. Requirement	Goal
Hor. Resolution	km	100 - 200	<50
Vert. Resolution	km	1 - 3	0.2
Time Resolution	h	24 / monthly	<1
Uncertainty	%	<10 / 1-3	1
Stability	% dec^{-1}	3	<1

To help investigate the ozone in the UTLS and gain confidence in Chemistry Climate Models (CCMs), a new product will be generated within Phase 3 of ESA Ozone_cci+, specifically focusing on the UTLS region using observations by limb sensors. To understand the user needs of the community investigating the UTLS, we created a survey and reached out to members of the OCTAV-UTLS (https://www.octav-utls.net) and the TPChange (https://tpchange.de) communities in March 2025. The primary requirements of the five replies agreed very closely and can be found in Table 4.

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 in 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 the 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.

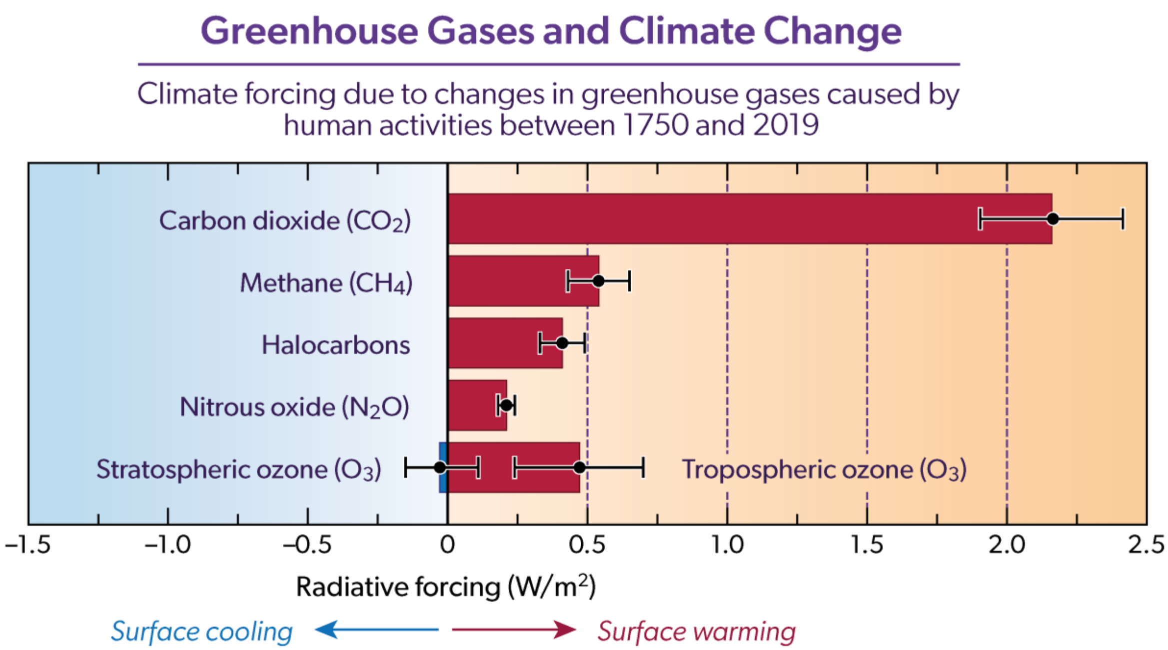

Figure 1: Radiative forcing of greenhouse gases and ozone depletion. Human activities since the start of the Industrial Era (around 1750) have caused increases in the atmospheric abundance of greenhouse gases (GHGs). Rising levels of GHGs lead to an increase in the radiative forcing (RF) of climate by trapping infrared radiation released by Earth's surface. Here, values of RF are for the time period from 1750 to 2019 and are expressed in units of watts per square meter (W/m2); black whiskers on each bar show uncertainties. Positive values of RF (shown in red) contribute to global warming and negative values (shown in blue) contribute to climate cooling. The largest positive RFs are due to carbon dioxide (CO2), methane (CH4), tropospheric ozone (O3), halocarbons, and nitrous oxide (N2O). Halocarbons include all ozone-depleting substances, hydrofluorocarbons, and a few other gases. The RF due to ozone is shown as the separate response to changes in ozone within two layers of the atmosphere: the troposphere and stratosphere. Tropospheric ozone increases result from the emission of air pollutants and lead to a positive RF whereas stratospheric ozone depletion leads to a small RF that could be negative or positive. Figure and caption taken from Salawitch et al. (2023), Figure Q17-1.

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 in 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 2018 with a second phase in 2022 (CCMI-2022). 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 basis 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, making reliable scientific conclusions difficult. Merged data sets are often based on data assimilation techniques, i.e. techniques built 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) is 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 the tropospheric ozone column difference between the individual CCMI models and the OMI-MLS dataset for the year 2005. In the multi-model mean, the CCMs tend to overestimate the amount of ozone; however, there is a large spread between the models.

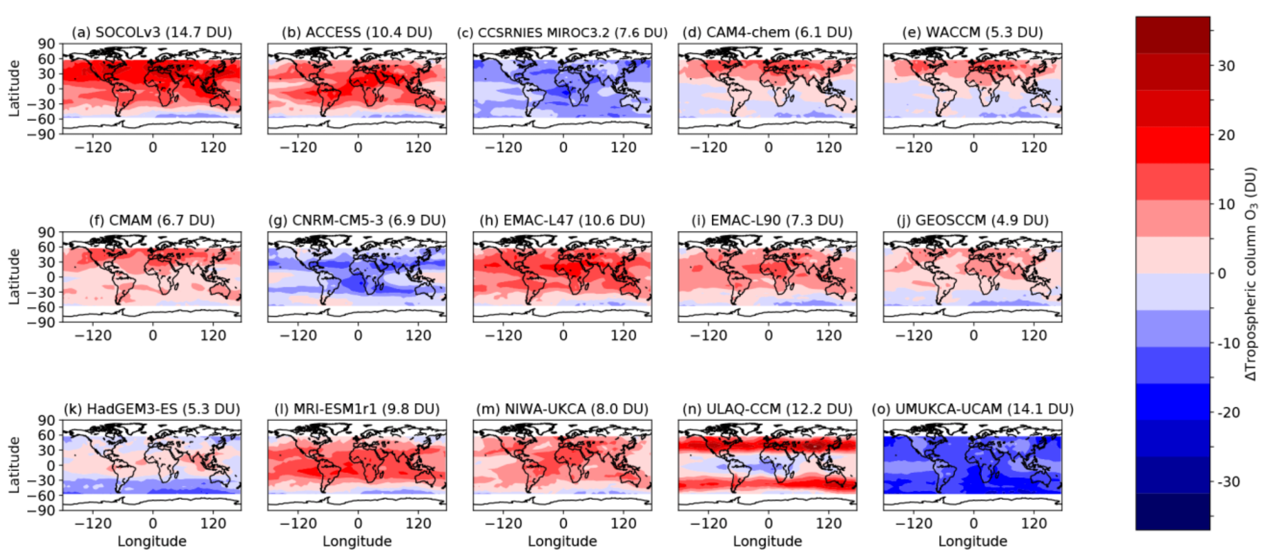

Figure 2: Difference between annual-mean year 2005 tropospheric column ozone in CCMI models compared with OMI-MLS, i.e. model minus OMI-MLS. The root-mean-square error for each model compared with OMI-MLS is indicated in the title. Figure and caption taken from Revell et al. (2018), Figure 7.

Figure 3 compares the tropospheric ozone column zonal mean trends of the CCM CESM2-WACCM6 (Community Earth System Model 2 – Whole Atmosphere Community Climate Model Version 6; Gettelman et al., 2019) over the time periods 1979-2005 and 2005-2014 with the satellite products of TOMS and OMI-MLS, respectively. The agreement with OMI-MLS is better than for TOMS and shows the largest differences in the latitude bands northwards to the equator.

Figure 4 illustrates why Averaging Kernels (AK) have to be considered when comparing CCM model output with satellite data, especially from nadir sounders. Shown is the difference in the tropospheric column between two independent CCM models, EMAC and CMAM, monthly averaged from pole to pole. When the AKs are included, the differences are present everywhere. Even in areas of the largest differences without AKs, the difference can change the sign (compare (c) and (e) northward of 60° N.

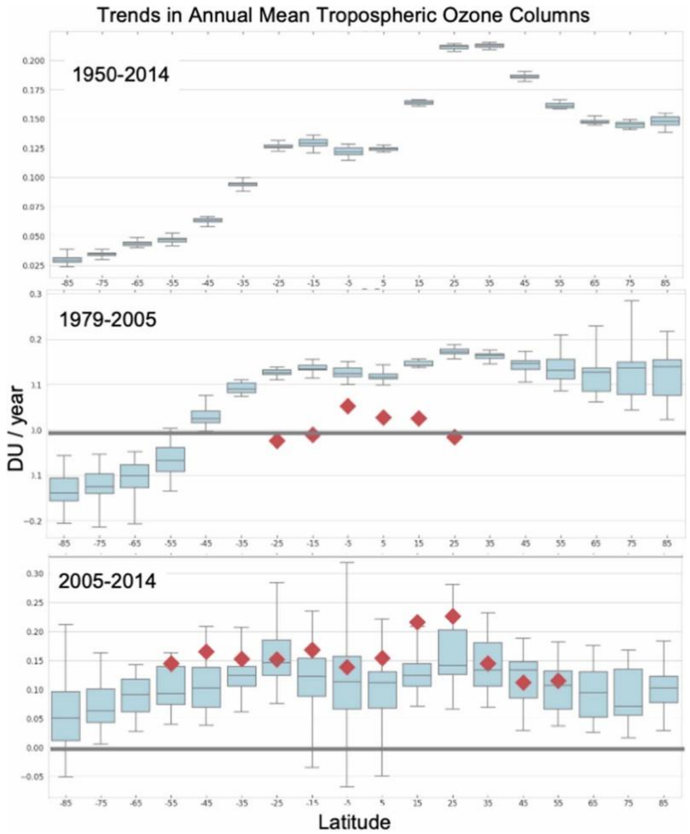

Figure 3: Increasing tropospheric column ozone trends (DU yr^{-1}) in the latter half of the 20th Century, and comparison to trends derived from the satellite record. Shown are the distribution of trends across the 15-member CESM2-WACCM6 initial-condition ensemble (blue box denotes inter-quartile (25^{th}–75^{th} percentile) range; whiskers denote 2-sigma range) within 10° latitude bands from 1950 to 2014 (top), 1979 to 2005 (middle), and 2005 to 2014 (bottom). Red diamonds denote the satellite-derived trends from TOMS (middle) and OMI-MLS (bottom). Different tropopause definitions are used for consistency with retrieval approaches from TOMS (100 hPa pressure surface) versus OMI-MLS (thermal lapse rate, also used for 1950–2014 period). Figure and caption taken from Fiore et al. (2022), Figure 6.

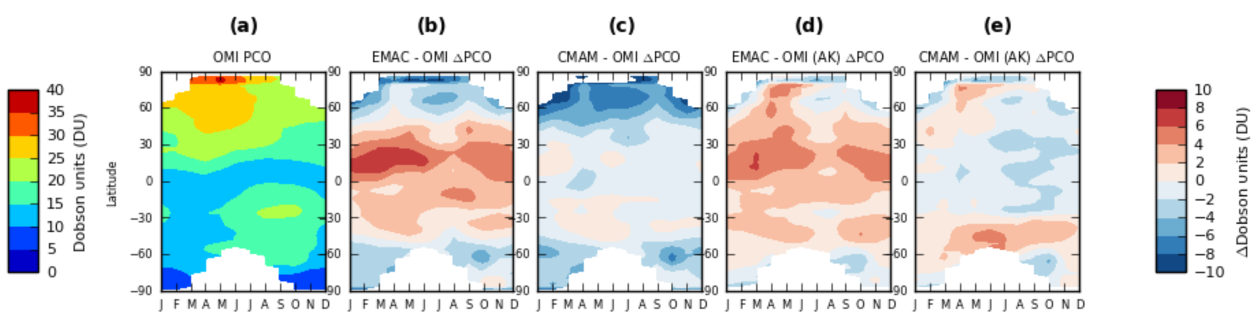

Figure 4: Zonal-mean monthly averaged 1000–450 hPa (0–5.5 km) sub-column O3 (DU) for 2005–2010 from (a) OMI, (b) EMAC minus OMI without AKs, (c) CMAM minus OMI without AKs, (d) EMAC minus OMI with AKs and (e) CMAM minus OMI with AKs. Figure and caption taken from Williams et al. (2019) figure 2.

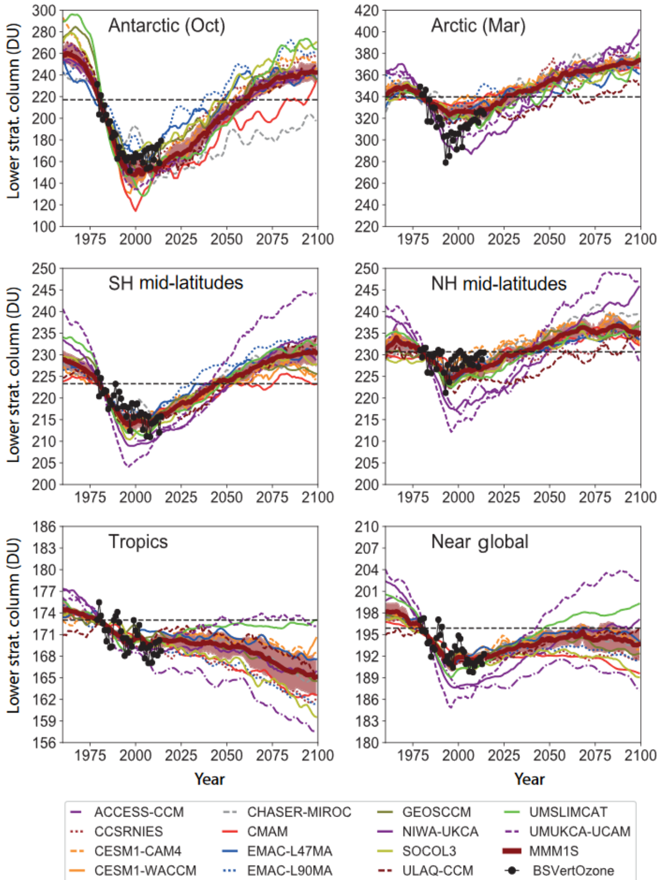

Figure 5: Evolution of partial column ozone (DU) for the lower stratosphere (tropopause – 10 hPa) from the REF-C2 simulations from 14 individual models, along with the MMM1S. Also shown are estimates of the partial column from the Bodeker Scientific Vertical Ozone (BSVertOzone) database, which is based on a compilation of satellite, balloon, and ground-based measurements (Bodeker et al., 2013). Figure and caption taken from Dohmse et al. (2018), Figure 5.

Moving higher up into the lower stratosphere, Figure 5 compares the partial column ozone evolution in six latitude bands between the CCMI simulations of REF-C2, the transient reference simulation from 1960 to 2100 (Morgenstern et al., 2017), and the BSVertOzone database. MMM1S is defined as the multi-model mean over all models that are within 1-sigma of the mean in each year. While the evolution until 2100 for all models shows a similar behaviour, especially in the Arctic region, the models tend to overestimate the amount of ozone in the lower stratosphere. A similar analysis for the middle and upper stratosphere can be found in the reference mentioned in the figure caption.

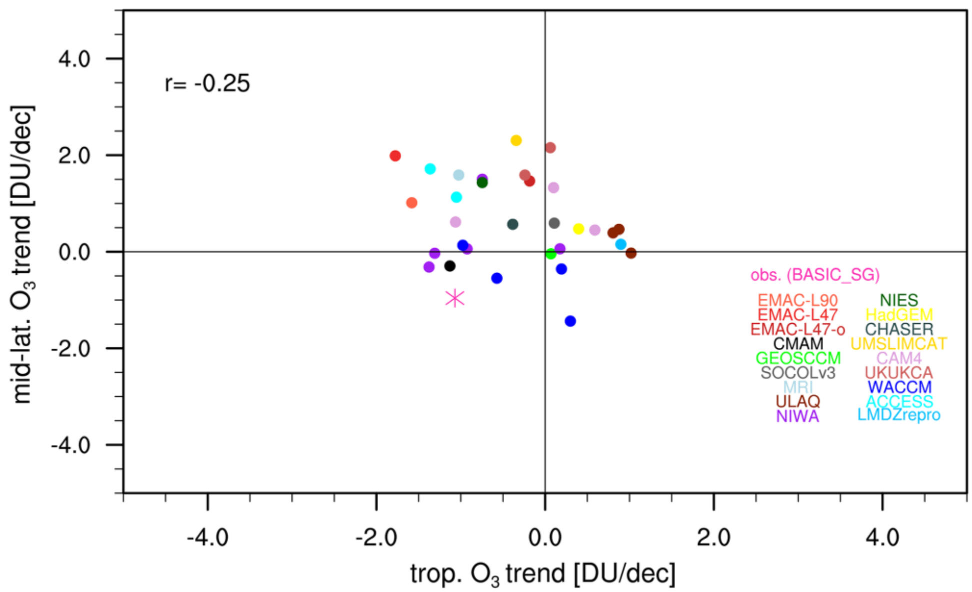

Figure 6: Inter-model correlation between tropical (20° S–20° N) and northern mid-latitude (30°–50° N) lower stratospheric ozone column trends, calculated over the period 1998–2018 for 31 CCMI REF-C2 simulations. All ensemble members of a particular model are shown in the same colour. The observational ozone trends ($BASIC_{SG}$) are included as a star. Figure and caption taken from Dietmüller et al. (2021), Figure 3.

Figure 6 shows the partial column trends in the lower stratosphere (LS) in the tropical and northern hemisphere mid-latitude region of the CCMI simulations. The trends are compared to the $BASIC_{SG}$ dataset presented in Ball et al. (2018). It merges the Stratospheric Water and Ozone Satellite Homogenized database (SWOOSH) (Davis et al., 2016) with the Global OZone Chemistry And Related trace gas Data records for the Stratosphere (GOZCARDS) (Froidevaux et al., 2015) using the BAyeSian Integrated and Consolidated (BASIC) method (Ball et al., (2017). The CCMI models overestimate the LS ozone column trends in the mid latitudes. Most models show a positive trend in the mid latitudes and only a few show a negative trend in both latitude regions.

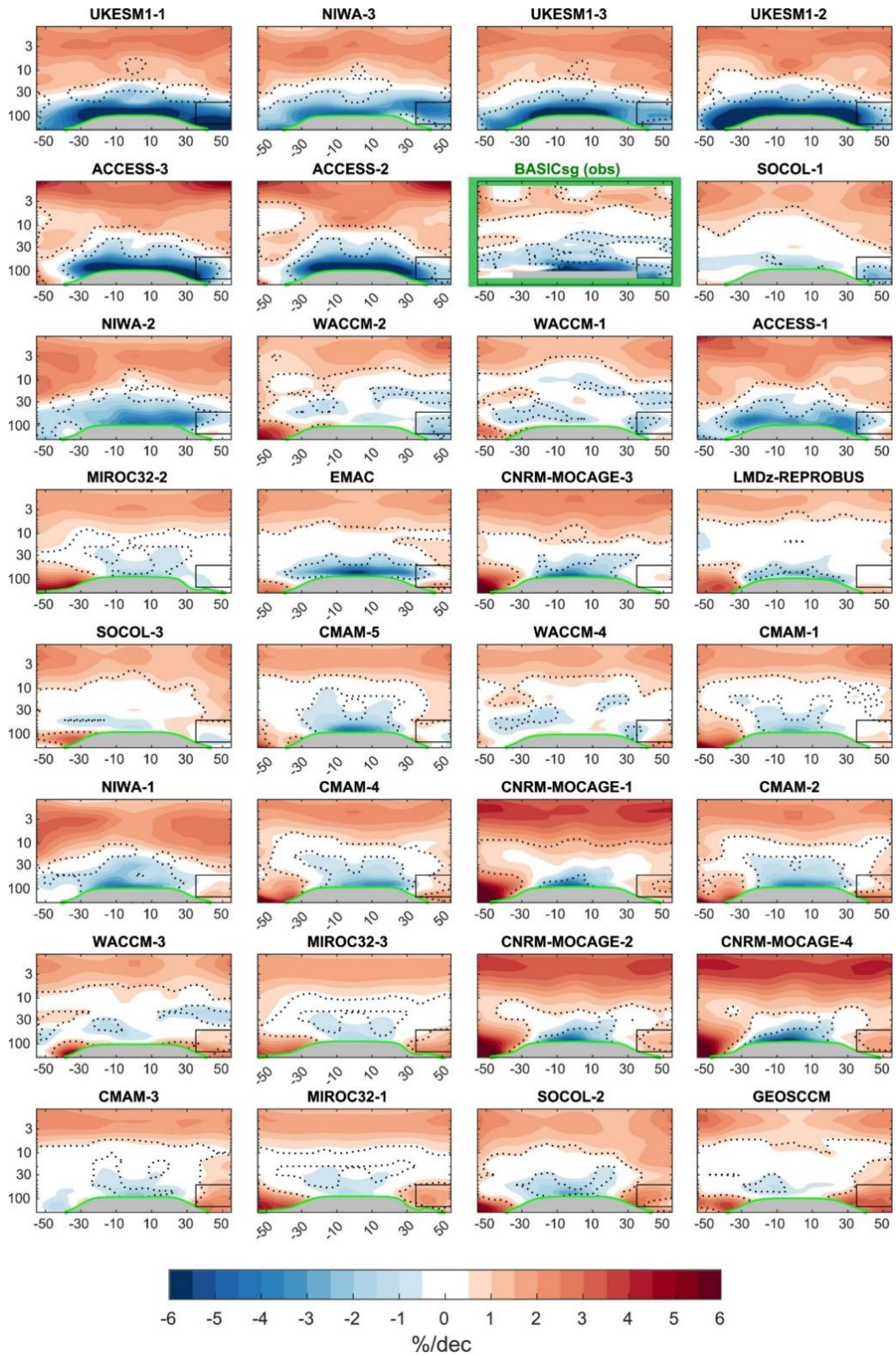

Figure 7: Latitude-pressure cross-section of the relative ozone trend (% per decade) between 1998–2018 from the BASIC$_{sg}$ observational data and all REF-D1 simulations. The relative trend is calculated with respect to the 1998–2018 climatology. The simulations are ordered by the partial column ozone trend value in the northern midlatitudes lower stratosphere region (black boxes; 35°–55°N, 50–150 hPa). The numbers in the panel titles indicate the ensemble member. The WMO tropopause is indicated by the thick green line. Black dashed contours denote statistically significant trends at 95% confidence level (p-value <0.05). The green box marks the observations panel. Figure and caption taken from Benito-Barca et al. (2025), Figure 1.

In Figure 7, the $BASIC_{SG}$ data record is used to study ozone trends over the last twenty years in the stratosphere in the latitude-pressure plane. The analysis is done with all CCMI-2022 hindcast reference simulations REF-D1 (https://blogs.reading.ac.uk/ccmi/ccmi-2022). The largest differences between the CCMI models are found in the lowest regions of the stratosphere. Around the tropics, the trends are negative or statistically not significant. But in the higher latitudes, the models disagree even in the sign of the trend. This emphasises the UTLS region as a region of large uncertainty and a region where we still have to improve our understanding and therefore need more and better data products to evaluate the CCMs.

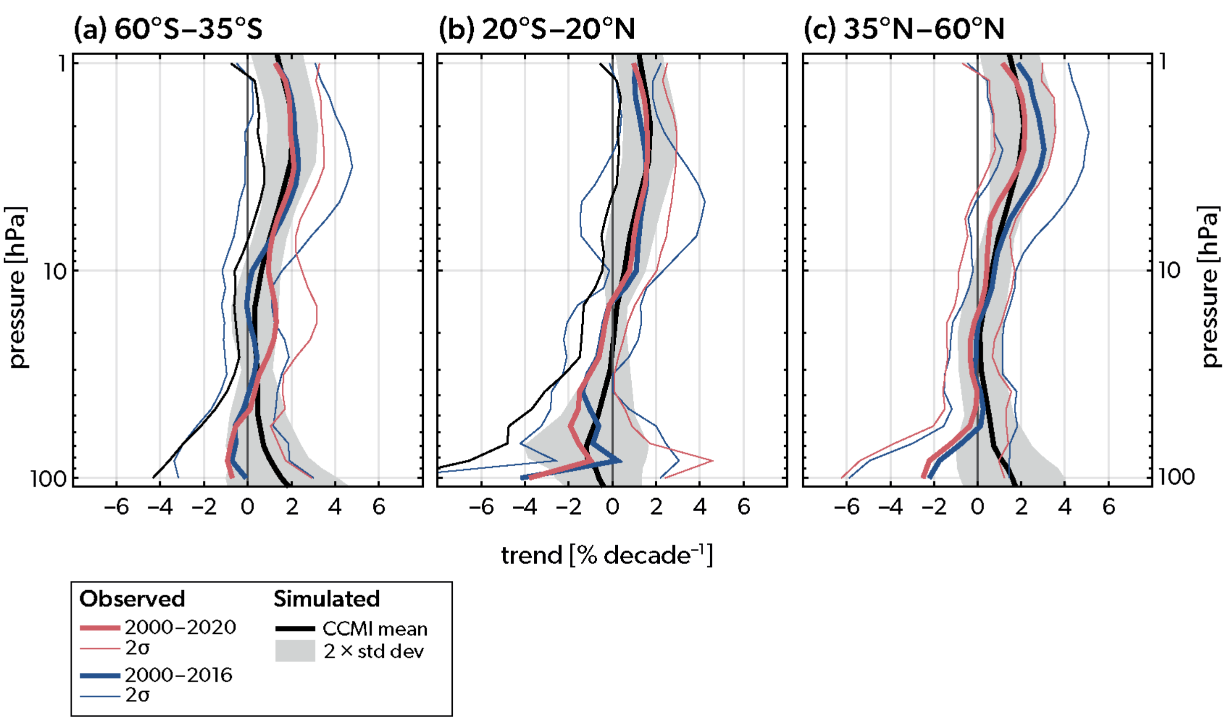

Figure 8: Comparison of simulated and observed post-2000 ozone trend profiles for the latitude bands 35–60°S (left panel), 20°S–20°N (center panel), and 35–60°N (right panel). Observed trends from the 2018 Ozone Assessment (the period 2000–2016) are shown in blue, and updated results for the period 2000–2020 are shown in red, with the trend values based on combining different merged satellite datasets and their 2σ uncertainties, all estimated using the method outlined by SPARC/IO3C/GAW (2019). The black line is the multi-model mean trend calculated from 16 CCMI-1 REF-C2 simulations (Morgenstern et al., 2017), with the spread of the individual model trends (±2 standard deviations) indicated by the gray shading. [Adapted from Godin-Beekmann et al., 2022.]. Figure and caption taken from WMO Ozone Assessment report 2022, Figure 3-12.

Figure 8 displays trends in the stratosphere by an ensemble of CCMI simulations in three latitude bands and observed trends reported in the 2018 and 2022 Ozone Assessments, based on merged satellite datasets. Simulated and observed trends differ mainly in the mid-latitudes and show an improvement in the newer satellite products. The CCMI models agree quite well with the observations; differences are largest in the lower stratosphere, which agrees with Figure 7. A similar analysis can be further found in Benito-Barca et al. (2025).

All these different examples of applications show that the community needs long, consistent datasets to analyse trends and that observations, especially in the stratosphere, are widely used by the ozone modelling community. The largest uncertainties are currently found in the lower stratosphere, as a result of the large, natural interannual variability and the lower signal to noise ratio for limb sensors. Tropopause-referenced satellite products would eliminate a part of the natural variability and therefore provide more robust ozone trends (Thompson et al, 2021) and help with the otherwise large spread of trend signs by climate models.

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.

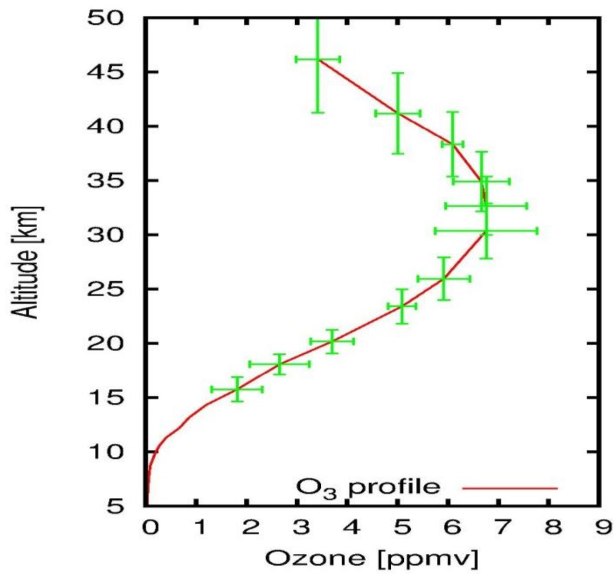

Figure 9: Sketch illustrating an ozone profile and the reporting of errors.

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 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 better understand 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 homogenised/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 characterised.

Table 5: 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. GCOS-245 (2022) requirements were based on this requirements table.

Quantity	Driving Research topic	Geographical zone		
		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)	(1995 -)	(1995 -)	(1995 -)
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, and regime studies.

Table 6: 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 (UTLS). CCMs explicitly resolve the troposphere and the stratosphere. For the nadir-viewing instruments, the intrinsic coarser vertical resolution (~6 km) is acceptable. Nadir ozone profile observations typically have a very good horizontal coverage. Partial column 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 UTLS region is of particular importance for the Earth's climate system, including surface climate. The temporal resolution should agree 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:

- The tropopause is defined by the (pressure) altitude using the WMO temperature criterion ($< 2\ K\ km^{-1}$) or the (pressure) altitude above which the ozone mixing ratio continues to exceed 150 ppbv.
- 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 homogenised/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 characterised.

Table 7: 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 UTLS is located at about 6-20 km altitude, and the middle and upper stratosphere extends between 20-50 km altitude. The required coverage is global. Achievable and future target requirements are given, separated by a '–'. The first number is the future target. GCOS-245 (2022) requirements were based on this requirements table..

Quantity	Driving Research topic	Height range		
		Troposphere	UTLS	Middle + Upper Stratosphere
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)	(1995 -)	(1995 -)	(1995 -)
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 8: 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 UTLS. 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 agree 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:

- The tropopause is defined by the (pressure) altitude using the WMO temperature criterion (< 2 K km^{-1}) or the (pressure) altitude above which the ozone mixing ratio continues to exceed 150 ppbv.
- 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 homogenised/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 characterised.

The ozone variability in the UTLS is large due to latitude-dependent variations in the tropopause height as well as the annual cycle. For ozone trend detection in the UTLS region, it is beneficial to use a tropopause-referenced vertical coordinate (Thompson et al, 2021). The tropopause-referenced product should cover two solar cycles for robust trend analyses and should mirror the horizontal and vertical resolution of climate models in the UTLS, of the order of 200 km horizontally and 1 km vertically. Additional information has to be available, such as the exact definition of the tropopause used as a reference, as well as its height and pressure information.

Table 9: 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 UTLS extends from about 6 km to the tropopause (UT) and from there to about 20 km (LS). The middle and upper stratosphere extends from about 20 km to 50 km altitude. The required coverage is global. Achievable and future target requirements are given, separated by a '–'. The first number is the future target. GCOS-245 (2022) requirements were based on this requirements table.

Quantity	Driving Research topic	Height range	
		UTLS	Middle + Upper Stratosphere
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 % dec^{-1}	1 – 3% / decade

Table 10: 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
Tropopause information included?	Yes, per profile; important for the tropopause-referenced product (altitude and pressure)
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 for tropospheric products based on the nadir profile retrievals are found in Section 4.3 and repeated in Table 11. 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 and continuing to this day with several sensors based on an evolved GOME instrument design.

Table 11: Product requirements for CCD- and LNM-based tropospheric ozone 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. Values are based on GCOS-245 (2022).

Quantity	Driving Research topic	Tropospheric column
Horizontal resolution	Regional differences in tropospheric ozone burden (radiative forcing); Seasonal cycle and interannual variability; Short-term variability	5 – 100 km
Vertical resolution	Height dependence of evolution of tropospheric ozone burden (radiative forcing); Seasonal cycle and interannual variability; Short-term variability	n/a
Observation frequency	Evolution of tropospheric ozone burden (radiative forcing); Seasonal cycle and interannual variability; Short-term variability	Daily – weekly
Time period	Evolution of tropospheric ozone burden (radiative forcing)	(1995 -)
Uncertainty	Evolution of tropospheric ozone burden (radiative forcing)	5 – 15 %
Uncertainty	Seasonal cycle and interannual variability; Short-term variability	5 – 15 %
Stability	Evolution of tropospheric ozone burden (radiative forcing); trends	1 – 3 % dec^{-1}

Table 12: 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
Top level information included?	Yes, per pixel (altitude and pressure)
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 *Geostationary satellite tropospheric ozone product*

Within Phase 3 of Ozone_cci+, the RAL nadir UV ozone profile scheme will be applied to obtain information on tropospheric ozone from the relatively new geostationary UV/visible sounders GEMS (launched February 2020) and TEMPO (launched April 2023). The operational code developed by RAL (Siddans et al., 2024) for the analogous Sentinel-4 (S4) UVN sounder (planned for launch in July 2025) will be used.

Compared to the UV sounders in polar orbit (e.g. GOME-2, OMI, S5P), these three geostationary instruments do not measure in the Hartley band spectral range (below ~300 nm) and therefore lack profile information in the stratosphere. Information on total and tropospheric ozone is still available from the Huggins bands (310-340 nm).

User requirements for tropospheric ozone from Sentinels-4 and 5 are defined in the ESA S4/5 Mission Requirements and Traceability Document (Langen et al. 2017), based on the user requirements established for Copernicus (Kelder et al. 2006). These are summarised in Table 13 below.

Table 13: Product requirements for geostationary tropospheric column data, based on the Sentinel 4/5 MRTD (ESA, 2017). Where numbers are given as "a / b", the first is the target requirement and the second is the threshold requirement. In the left-hand column, the codes refer to the target applications: Letters A, B, C refer respectively to areas "Stratospheric Ozone and Surface UV", "Air Quality" and "Climate". Numbers refer to needs (within these areas) for (1) protocol monitoring and treaty verification; (2) near-real-time applications; (3) scientific assessment.

Application	Horizontal resolution	Revisit time	Uncertainty
B1, B2, B3	5 km / 20 km	0.5 h / 2 h	25 % / 40 %
A2, A3	10 km / 50 km	6 h / 3 days	25 % / 40 %
C1	10 km / 50 km	12 h / 3 days	25 % / 40 %
C2, C3	10 km / 50 km	6 h / 3 days	25 % / 40 %

All three of the geostationary sounders observe with at least 8 km spatial resolution and hourly sampling, and so meet the horizontal resolution and revisit time requirements.

For Sentinel-4 processor development (Siddans, 2024), the uncertainty requirement was relaxed to 25 % (goal) / 40 % (threshold), for observing conditions with solar zenith angle < 60°, view zenith angle < 60° and assuming the cloud fraction is less than 20 %. We adopt this relaxed requirement also for GEMS and TEMPO.

In this context, "tropospheric column" is the estimated layer-averaged mixing ratio, determined by integrating the retrieved ozone profile between the surface and 450 hPa and normalising by the corresponding air layer number density. The uncertainty requirement is to be understood as applicable after allowance has been made for the vertical sensitivity of this quantity to the true vertical distribution of ozone (using the averaging kernels).

4.7 *Recommendations on Level-1 data product from the 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.

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