TITLE:

Ozone-cci

User Requirement Document (URD)

Date: 21-11-2011

Version: 2.1

Phase 1, Task 1

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CRG: DLR-PA, UCAM
EOST: DLR-IMF, BIRA, RAL, IUP, FMI, LATMOS

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

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1 Introduction

1.1 Purpose

This User Requirement Document of the Ozone_cci project is summarising the user requirements for three ozone ECV (Essential Climate Variable) products, total ozone columns, 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 three 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), the CMUG, IGACO(2004), and the WMO rolling requirements. The Climate Research Group (CRG) of the Ozone_cci project has interpreted these requirements and “translated” them to the requirements for the data products that will be created in the Ozone_cci project. The scientific rationale behind the selection of the Ozone_cci data products is also given as appropriate throughout the document.

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, nadir ozone profile, and limb ozone profile) the quantitative ozone data requirements, including accuracy, 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 3 we describe the various existing requirements on ozone products for climate research, especially the requirements from GCOS and CMUG. In Chapter 4 the CRG, responsible for this document, is introduced. Chapter 5 introduces the scientific rationale for the Ozone_cci products and in Chapter 6, the final requirements, their rationale and their traceability are given.

2 Applicable Documents and references

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

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)

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)

WMO rolling requirements: Based on WMO-TD No. 1052, SAT-26 and on-line available from http://www.wmo.int/pages/prog/sat/Requirements/Observational-requirements_web.xls

3 Available ozone requirements

3.1 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. Among others GCOS focuses on satellite and *in situ* observations for climate in the atmospheric domain. 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.

Environmental climate variables (ECVs) are required to improve our understanding of the climate system. In conjunction with numerical modelling they support projections of the climate system. In the context of the "Ozone_cci", a better understanding of natural and anthropogenic forcings affecting the atmospheric ozone distribution will be developed. 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 accuracy 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.

"Ozone_cci" will provide significant contributions to GCOS. Long-term consolidated data sets based on different satellite instruments will be the foundation for improved model quality evaluation, allowing a more detailed insight into individual dynamical and chemical processes. For example, so far 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.

Table 1: The GCOS target requirements on ozone based on GCOS-107 (pages 23+24).

Accuracy	10% (troposphere) 20% (stratosphere)
Horizontal resolution	5-50 km (troposphere) 50-100 km (stratosphere)
Vertical resolution	0.5 km (troposphere) 0.5-3 km (stratosphere)
Observation frequency	3-hourly
Stability	1% (troposphere) 0.6% (stratosphere)

The horizontal and vertical resolution and observation frequency are mainly justified on the commonly used (standard) resolution of currently available and used model systems (e.g. Morgenstern et al., 2010, for the CCMs). For the troposphere regional models are often used which have a much higher horizontal resolution. The required horizontal resolution (i.e. 50-100 km) is too high; it would be sufficient to have 100-300 km.

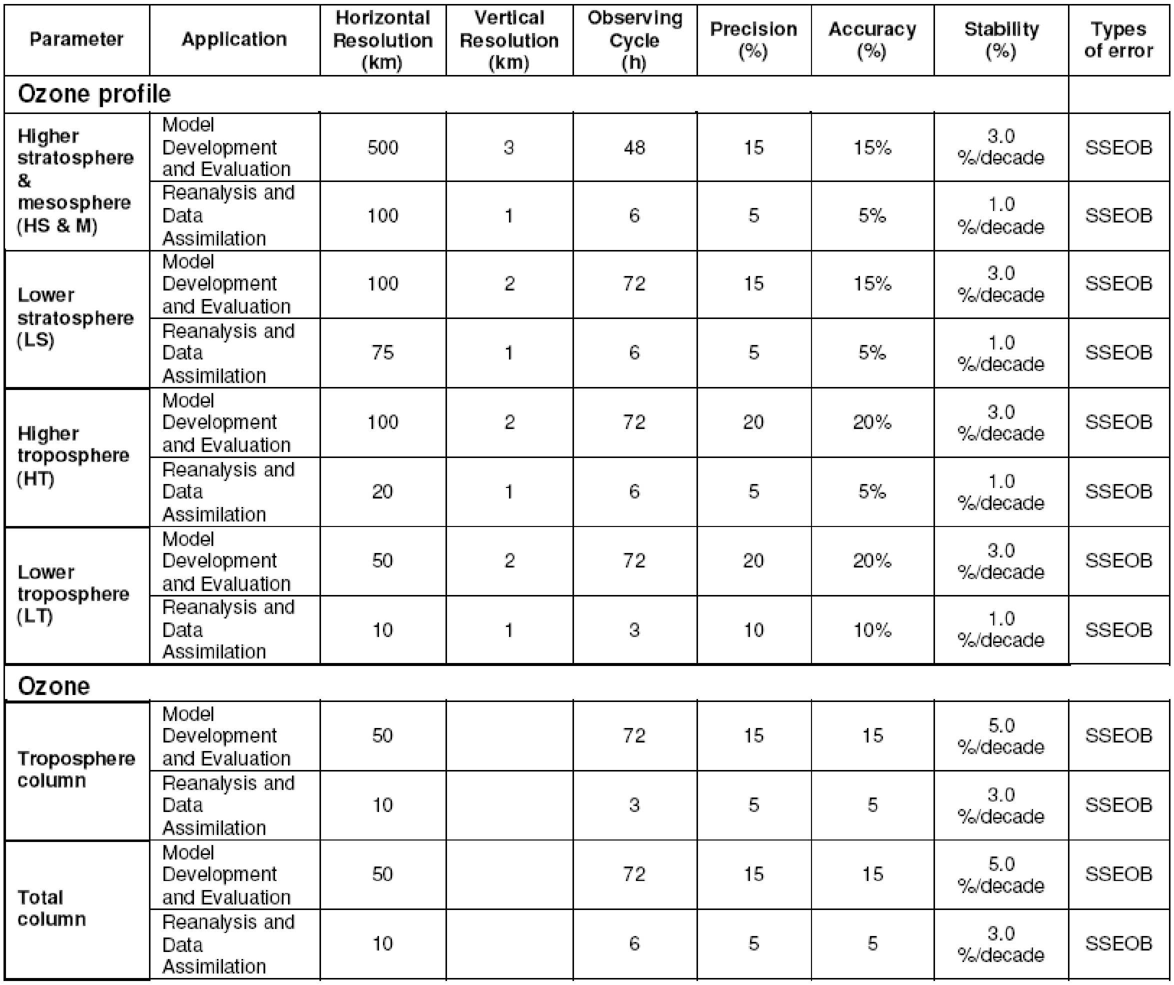
For example, a monthly mean ozone data set (mixing ratios) on a horizontal 2x2deg. grid with a vertical resolution of 2 km covering multiple decades would be an extremely valuable tool for model validation, in particular if meta-data is provided like the error in each bin, a quality marker (maybe the number of cloud free measurements used), etc.

It should be noted that the GCOS target requirements also refer to 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 future targets.

3.2 Climate Modelling User Group (CMUG)

The main objective of the Climate Modelling User Group (CMUG) is to provide guidelines within ESAs Climate Change Initiative to the currently eleven sub-projects 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. Therefore, the Climate Research Group (CRG) within "Ozone_cci" will help to define the user requirements from the modeller's point of view as well as necessary specification for the required data products. They will help to integrate and assess the global ozone data products in the context of numerical models. Moreover they will 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

3.3 IGACO observational requirements on ozone

The IGACO 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; TTOC = tropospheric total ozone column.

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

3.4 WMO rolling requirements on ozone

The WMO rolling requirements (downloaded December 2010) are available from: http://www.wmo.int/pages/prog/sat/Requirements/Observational-requirements_web.xls

Table 4: WMO rolling requirements on ozone, based on WMO-TD No. 1052, SAT-26

"Requirement from Atmospheric Chemistry"	Horizontal Resolution (km)			Vertical Resolution (km)			Observing Cycle (h)			Delay of availability (h)			Accuracy		
Parameter name	Goal	B	Th	Goal	B	Th	Goal	B	Th	Goal	B	Th	Goal	B	Th
Ozone profile – Higher stratosphere & mesosphere (HS & M)	50	107.7	500	1	1.7	5	3	7.6	48	72	95.5	168	5 %	8.5 %	25 %
Ozone profile – Higher troposphere (HT)	50	107.7	500	1	1.7	5	3	11.5	168	72	95.5	168	3 %	5.6 %	20 %
Ozone profile – Lower stratosphere (LS)	50	107.7	500	1	1.7	5	3	11.5	168	72	95.5	168	3 %	5.6 %	20 %
Ozone profile – Lower troposphere (LT)	50	107.7	500	1	1.7	5	3	11.5	168	72	95.5	168	3 %	5.6 %	20 %
Ozone profile – Total column	25	39.7	100				6	12	48	3	11.5	168	6 DU	9 DU	20 DU

"Requirement from Atmospheric Chemistry"	Confidence	Application		
Parameter name		Use	Remarks	Source/Validation
Ozone profile – Higher stratosphere & mesosphere (HS & M)	Firm	Atmospheric chemistry	Strat chem/clim, Rad effects/clim, Ozone chem	24/5/2002, WMO TD No. 1052, SAT-26
Ozone profile – Higher troposphere (HT)	Firm	Atmospheric chemistry	Trop chem/clim, Rad effects/clim, Ozone chem	24/5/2002, WMO TD No. 1052, SAT-26
Ozone profile – Lower stratosphere (LS)	Firm	Atmospheric chemistry	Oxid cap, Rad effects/clim, Strat climat, O3 chem	24/5/2002, WMO TD No. 1052, SAT-26
Ozone profile – Lower troposphere (LT)	Firm	Atmospheric chemistry	Trop chem/clim, Rad effects/clim, Oxid cap	24/5/2002, WMO TD No. 1052, SAT-26
Ozone profile – Total column	Firm	Atmospheric chemistry	UVB pred/anal, Dynamics	24/5/2002, WMO TD No. 1052, SAT-26

3.5 Across-ECV requirements and international climate modelling

Potential synergy is foreseen for the combined use of different ECVs, including ozone, in climate model evaluations. 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 coming years, and will lead to more sophisticated process-based Earth-System validation exercises. The ozone ECV products will be an integral part of these, e.g. related to changes in transport regimes in troposphere and stratosphere, and stratosphere-tropopshere 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.

The stratospheric ozone layer still is and has been an important research topic for the last 25 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 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, 2011).

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).

The recent 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 not well understood. 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.

In conclusion, 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.

4 Ozone Climate Research Group

4.1 Introduction

The targeted specialised climate research community aims at the evaluation of chemistry-climate models (CCMs) with particular focus on long-term numerical simulations using CCMs for the detailed investigation of model feedbacks between ozone chemistry, ozone depleting substance (ODS) trends, and climate. This research community is intensively involved in international activities of climate research including stratospheric and tropospheric responses and feedbacks.

The climate research community is represented within the project by the Climate Research Group (CRG), which consists of Climate research experts specialised in the modelling of global climate and its feedback with chemistry. It is led by Dr. M. Dameris from DLR.

- DLR: the team at DLR-PA, represented by M. Dameris, has been developing coupled chemistry-climate models (CCMs) since about 20 years. Scientific investigations have been carried out focussing on individual dynamical and chemical processes in the atmosphere and their feedback mechanisms.
- UCAM: the UCAM team represented by P. Braesicke has acknowledged expertise studying the interactions between atmospheric composition and climate, with particular emphasis on modelling the stratospheric ozone layer, stratosphere-troposphere exchanges, and attributing stratospheric (post-volcanic) ozone changes.
- KNMI: the modelling team at KNMI, represented by P. van Velthoven and M. van Weele, has been acquiring extended knowledge of the climate system and its predictability through contributions to national and international efforts in the area of observation, monitoring and modelling of the climate system.

4.2 Ozone Climate Research DLR

So far DLR is analysing results derived from different simulations with the chemistry-climate model E39CA, concentrating on investigation related to the evolution of the stratospheric ozone layer in a changing climate: Transient simulations covering the period between 1960 and 2050 have been performed and validated against observations (e.g. Stenke et al., 2009; Garny et al., 2009; Loyola et al., 2009). In addition specific sensitivity studies in time-slice mode (i.e. fixed boundary conditions for single years) have been implemented to investigate specific mechanisms and processes (e.g. Garny et al., 2011). The results of E39CA simulations are considered in recent international evaluation exercises and assessment reports (e.g. SPARC CCMVal, 2010, WMO, 2011). In a first step, the output of E39CA will be used for evaluation purposes in "Ozone_cci".

Currently DLR is implementing a new model version, i.e. EMAC (Jöckel et al., 2006), which in parts built up on E39CA. EMAC contains a more detailed description of chemistry in the troposphere and improved parameterisations of sub-scale processes. Results of first EMAC simulations will be also used for comparisons with data products obtained in "Ozone_cci". Total column values as well as partial columns and ozone profiles derived from global observations are required for detailed investigations of short- and long-term variability of the ozone layer to better understand recent changes and to provide a more solid basis for prognostic studies. Moreover, this requires long-term, consistent data sets allowing statistically feasible analyses.

A focus of scientific research at DLR-PA is on investigations of chemistry-climate connections, the coupling of the troposphere and the stratosphere, long-term changes of atmospheric chemistry and dynamics in a changing climate, e.g. ozone recovery in the 21st century. In this project, among others the output of E39CA and EMAC will be used for evaluation purposes of the ozone ECVs.

E39CA

The coupled chemistry-climate model E39CA (Stenke et al., 2009) is an upgraded version of E39C (Dameris et al., 2005). The model top is centred at 10 hPa, with 39 levels between Earth surface and the model top; the horizontal resolution, on which the tracer transport, model physics and chemistry are calculated, is approximately 3.75°×3.75°. The chosen time step is 24 min.

The quality of E39CA has been intensively checked by evaluations with observations (e.g. Loyola et al., 2009; Stenke et al., 2009) and with respect to other CCMs (e.g. SPARC CCMVal, 2010). The results of E39CA have been used for assessment studies (e.g. WMO, 2011) and for a variety of process-oriented studies (e.g. Garny et al., 2009; 2011; Kremser et al., 2009; Kunze et al., 2010).

EMAC

The ECHAM/MESSy Atmospheric Chemistry (EMAC) model is a numerical chemistry and climate simulation system that includes sub-models describing tropospheric and middle atmosphere processes and their interaction with oceans, land and human influences (Jöckel et al., 2006). It uses the Modular Earth Submodel System (MESSy) to link multi-institutional computer codes. At DLR-PA, EMAC is the successor model system of E39CA. Currently, first long-term simulations are performed and model results are validated.

The core atmospheric model is the 5th generation European Centre Hamburg general circulation model (ECHAM5, Roeckner et al., 2006). EMAC is available in different horizontal and vertical resolution, e.g. the T42L90MA-configuration, i.e. with a spherical truncation of T42 (corresponding to a quadratic Gaussian grid of approx. 2.8°x2.8° in latitude and longitude) with 90 vertical hybrid pressure levels up to 0.01 hPa (approx. 80 km altitude).

4.3 Ozone Climate Research UCAM

UMUKCA (http://www.ukca.ac.uk/wiki/index.php/UKCA) as used by UCAM is a CCM based on the Met Offices Unified Model (UM). The UKCA acronym derives from the fact that the model is a United Kingdom's (UK) community model with chemistry (C) and aerosol (A). The first publication describing interactive integrations with this model system are Morgenstern et al. (2008; 2009). This model version participated in the SPARC CCMVal (2010) model intercomparison and contributed to the UNEP/WMO 2010 (2011) assessment of the ozone layer. This model superseded our earlier CCMs (e.g. Pyle et al., 2005) and has now been updated towards a new model version. Even though the name has not changed, the current UMUKCA is based on a newer version of the UM (currently 7.3; previously 6.1) and has benefitted from updates in parameterisations and functionalities. Note that the model is still very similar to the earlier version described in Morgenstern et al. (2009).

Currently, UMUKAC uses the 60-level version of the UM. The 60 levels go from the surface up to 84 km, with a resolution of 1km or below around the tropopause. Two horizontal standard resolutions are in use: N48 corresponding to an Arakaw-C grid of 3.75º×2.5º and N96, corresponding to a grid of 1.875º×1.25º (longitude×latitude). The dynamical core of the model is described by Davies et al. (2005). Unlike most climate models, the models formulation is non-hydrostatic and the vertical coordinate system is hybrid-height. Advection in the model is semi-Lagrangian (Priestley, 1993). Gravity wave drag comprises an orographic (Webster et al., 2003) and a parameterised spectral component (Scaife et al., 2002); the latter addresses subgridscale momentum transport from the troposphere to the middle atmosphere. Radiation follows Edwards and Slingo (1996) with 9 bands in the long- and 6 in the shortwave part of the spectrum. In the version considered here the model is run in an atmosphere-only mode forced with prescribed sea surface temperatures (SSTs) and sea ice. A comprehension ocean model is coupled, but will not be used in the framework of this project. The stratospheric chemistry is described in Morgenstern et al. (2009). Since the publication of this paper the photolysis model has been updated to Fast-Jx (Neu et al., 2007), the chemistry schemes for the stratosphere and the troposphere have been merged (optional), and the nudging capability (the option to constrain the model with observed meteorology) has been continuously developed and exploited (Telford et al., 2008 and 2009).

Apart from CCMVal runs, attribution studies for volcanic disturbances are performed (Telford et al., 2009), and support the attribution of observed ozone changes and variability. Sensitivity studies are used to establish important chemistry-climate interactions (Braesicke et al., 2010).

Deficiencies identified in integrations of the recent past are taken into account when interpreting projections of ozone throughout the 21st century.

Classic requirements: UMUKCA as currently used by UCAM is a chemistry-climate model capable of performing seasonal to centennial integrations. Integrations of the recent past are regularly performed with this model system (e.g. 1960 to present day). Validation of the modelled ozone includes assessments of the total ozone annual cycle, estimates of interannual variability, and trends in comparison to observations. In addition, latitude-height cross-sections of ozone mixing ratios are compared with well established satellite climatologies, usually concentrating on zonal and monthly mean distributions (Morgenstern et al., 2009). In addition, attribution studies for volcanic disturbances are performed (Telford et al., 2009), and support the attribution of observed ozone changes and variability. Deficiencies identified in integrations of the recent past are taken into account when interpreting projections of ozone throughout the 21st century. A joint assessment of many CCMs, including UMUKCA, can be found in the SPARC CCMVal Report and in WMO 2010 (see citations above).

Forthcoming requirements: In the future, a stronger emphasise will be on the comparison and validation of the vertical structure of ozone changes. This will require homogenised longitudinally resolved ozone products with a quality flag and binned in a suitable way (ozone being a function of longitude, latitude, height and time). Currently, the model can be run with a satellite and flight track emulator to sample the model like observations, also considering a vertical weighting (e.g. an averaging kernel), if required. At the moment this is done for case studies only, but a more general use is envisaged. Further exploitation of the nudged UMUKCA (Telford et al., 2008 and 2009) in conjunction with ERA-Interim is planned.

4.4 Ozone Climate Research KNMI

Ozone-climate interactions are being studied at the climate research department of KNMI, both from an observational and a modeling perspective. A major component of the ozone research at KNMI is the combination of observations and models, e.g. by data assimilation but also for the evaluation of the physical and chemical processes in numerical model simulations.

During the 1990s the TM3 global chemistry-transport model was developed and applied to e.g. assess the impact of emissions on climate forcing. Key research topics on ozone included stratosphere-troposphere exchange, ozone radiative forcing and the establishment of a climatology based on ozone sondes and satellite data (e.g. van Velthoven and Kelder, 1996; Bintanja et al., 1997; Fortuin and Kelder, 1998). The assimilation of satellite nadir ozone observations was first pioneered using the GOME and SCIAMACHY ozone observations and later operationalized (e.g. Eskes et al., 2003). In 1999 an ozone monitoring station was implemented by KNMI in Paramaribo, Surinam. It is part of the SHADOZ network and important for ozone satellite validation and studies focusing on tropospheric ozone at tropical latitudes (e.g. Valks et al., 2003). Ozone sondes are launched in the Netherlands since 1993. Nadir satellite observations of ozone columns and ozone vertical profiles and their assimilation are a major area of research in the Climate Observations division (e.g. van der A et al., 2009; de Laat et al., 2009). Chemistry-climate interactions of ozone, aerosols and their precursors are a major area of research in the Chemistry and Climate division. Reanalysis and scenario simulations as well as process studies on ozone are been performed (e.g. van Noije et al., 2004; 2006). The most important tool for current research on ozone-climate interactions is the EC-Earth/TM5 modeling framework (Hazeleger et al., 2010) which is described in more detail below. In a slightly different configuration TM5 is coupled to the ECMWF IFS atmosphere model in the MACC project providing near-real time atmospheric services including ozone in the framework of GMES.

The satellite data requirements for ozone are driven by the different type of research applications summarized above and include, off-line homogenized level-2 time series for process evaluations on time scales spanning from hours/days to months/years, and homogenized multi-instrument long-term data sets for ozone-climate interactions (Level 3 and Level 4). Near-real time level-2 product requirements as required within the MACC framework are not part of the user requirements for the Ozone_cci project.

EC-Earth

The EC-Earth consortium is a grouping of Earth system scientists from over ten European countries. EC-Earth is designed to bridge the gap between NWP and Earth system modeling and is used for basic research, for developing climate projections and predictions, and for delivering climate information to users. A central element of the strategy is to continually synchronize the atmosphere, land and ocean modules between the EC-Earth model and a reference configuration of the European Centre for Medium-Range Weather Forecasts (ECMWF) forecast system. To serve the climate science and prediction, the EC-Earth consortium couples various novel and improved Earth system modules to the model. The TM5 chemistry-transport model is the atmospheric chemistry and aerosol module of EC-Earth.

The NWP system of the ECWMF forms the basis of the EC-Earth model (hence the name EC-Earth). The atmospheric model of EC-Earth version 2, which is the current reference version, is based on ECMWF Integrated Forecasting System (IFS) cycle 31r1, corresponding to the current seasonal forecast system of ECMWF. The standard configuration (operationally 2011) runs at T159 horizontal spectral resolution with 62 vertical levels, but also exists in a configuration with 91 IFS levels for runs including the middle atmosphere (model top at 0.01 hPa). The model has recently been presented by Hazeleger et al. (2010) and is contributing to the Coupled Model Intercomparison Project (CMIP5) that provides input to the IPCC Fifth Assessment Report.

TM5

TM5 is a global chemistry-transport model with two-way nested grids. Regions for which high-resolution simulations are desired can be nested in the coarser global domain. The current TM5 model implementation is based on its predecessors (TM2, TM3, TM4) and is up-to-date in e.g. its chemistry and aerosol processing, advection scheme, and meteorological preprocessing of the wind fields (Krol et al., 2005). The TM5 model is developed and maintained jointly by the Institute for Marine and Atmospheric Research Utrecht (IMAU, The Netherlands), the Joint Research Centre (JRC, Italy), the Royal Netherlands Meteorological Institute (KNMI, The Netherlands), and NOAA ESRL (USA). In off-line mode the meteorological and surface fields which drive TM5 are based on operational forecasts or reanalysis fields from the ECMWF IFS model, but TM5 can also be run on-line as a module inside EC-Earth.ECMWF operational forecasts are currently run with ~16 km horizontal resolution and 91 layers. These data are interpolated to the TM5 grid(s) taking care that air mass is conserved. On the global domain TM5 is now mostly applied at 3x2 degrees (lon x lat) resolution. In zoom regions higher resolutions may be defined of e.g. 0.5x0.25 degrees. The most recent tropospheric-chemistry model version of TM5 is described in Huijnen et al. (2010). TM5 and its predecessors participated in various tropospheric chemistry multi-model intercomparisons over the last decade (e.g. Stevenson et al., 2006). Although the focus of TM5 is on tropospheric chemistry, stratospheric ozone variations are taken into account using either linearized chemistry, relaxation to an ozone climatology or satellite ozone observations (van der A, 2010). In the Ozone_cci project simulations using different EC Earth/TM5 model configurations on ozone will be evaluated.

5. Rationale for Ozone_cci products

This section introduces the rationale behind product developments in Ozone_cci. 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 extracted from the ITT (Section 5.1), representative CCM applications are briefly introduced (Section 5.2). Available ozone data products used for recent investigations are described in Section 5.3. Section 5.4 provides examples of intercomparison studies carried out for internationally organised evaluation exercises.

5.1 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 it 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 livings that breathe it and therefore it is often referred to as ‘bad’ ozone.

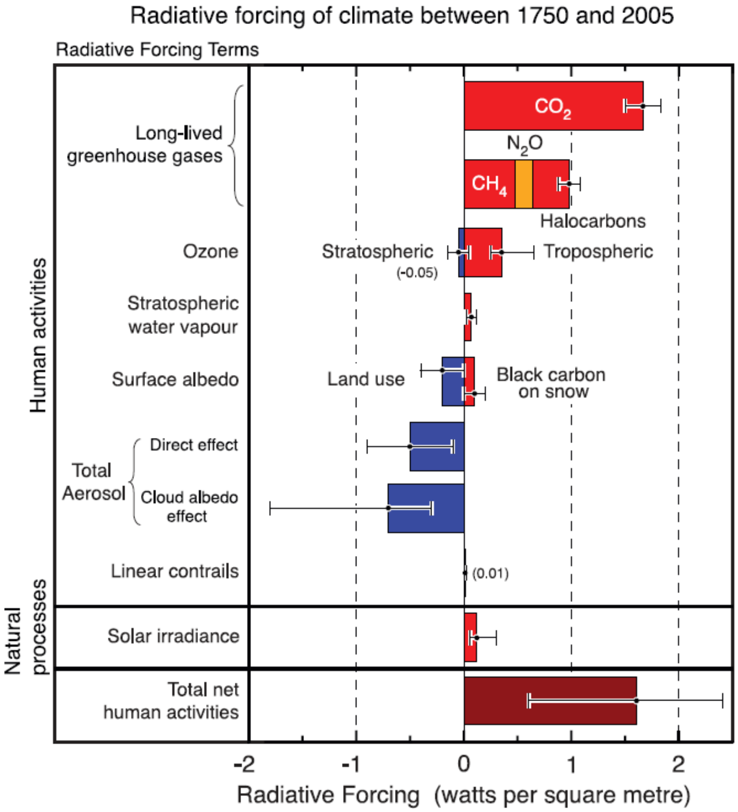


Figure 1: Summary of the principal components of the radiative forcing of climate change. All these radiative forcings result from one or more factors that affect climate and are associated with human activities or natural processes. The values represent the forcings in 2005 relative to the start of 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 2005 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 adapted from Figure 2.20 of IPCC Fourth Assessment Report: Climate Change 2007)

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 currently not well understood. 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.

5.2 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 are internationally coordinated by this activity. CCMVal aims 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. Coordinated model simulations have been carried out during the preparation phases of the two recent WMO Scientific Assessments of Ozone Depletion in 2006 and 2010 (WMO, 2007; 2011). The output of all participating CCMs (e.g. 18 for WMO, 2011) has been stored on compatible (spatial and temporal) grids (depending on the data product) and in a unified format (i.e. CF compliant netCDF) on a central data archive. Further information can be found at http://www.pa.op.dlr.de/CCMVal/ .

Section 5.4 provides examples of typical results for comparisons between model data and already available data from space-borne observations.

5.3 Observed ozone data

For recent 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 error (range of uncertainty) of such data products is often unknown, 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.

5.4 Linking modelled and observed ozone data

This section provides some examples for typical recent evaluations of ozone data derived from CCM simulations. Example are presented how available data products are used for evaluation purposes to identify strength and weaknesses of the models. Among others, the given examples should demonstrate that the evaluation of numerical models carried out so far with available data products is not sufficient and needs further action, in particular regarding improved data products derived from observations.

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). 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 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 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 time period before 1979. Here the observations are given without any indication of a range of uncertainty.

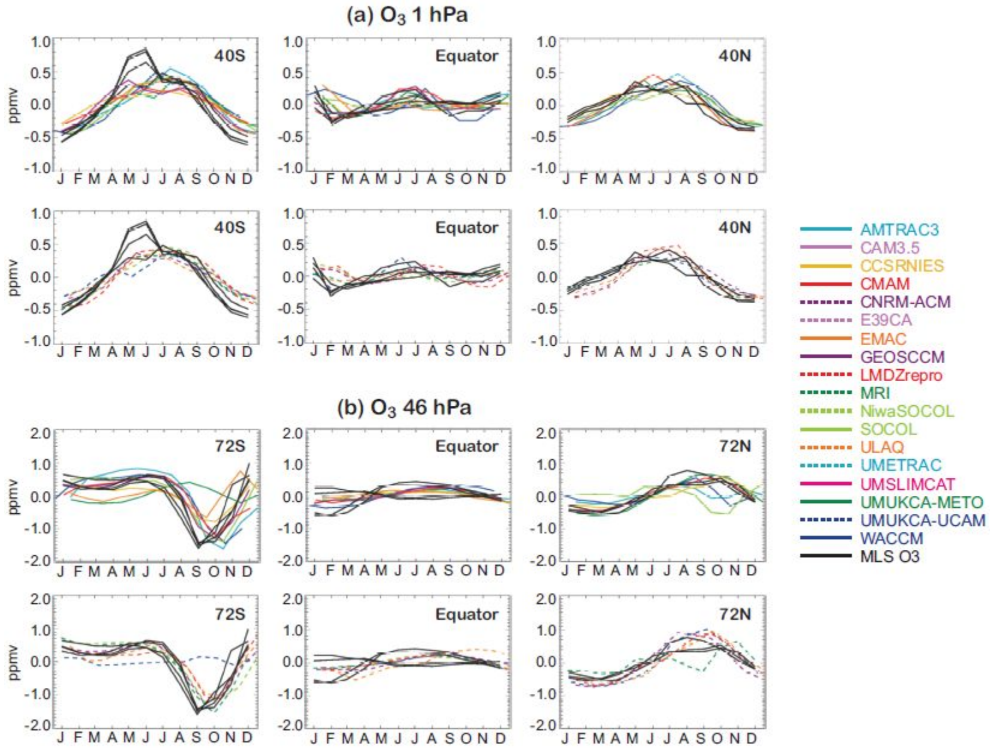


Figure 2: Anomalies of monthly mean ozone mixing ratios (in ppmv) at 1 hPa throughout the year, 40°S (left), Equator (middle) and 40°N (right) from several years of MLS observations (black lines) and for the CCMVal-2 CCMs (monthly zonal-mean ozone in the early 2000s from selected years; colour lines). MLS data are averaged for a six degree 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.)

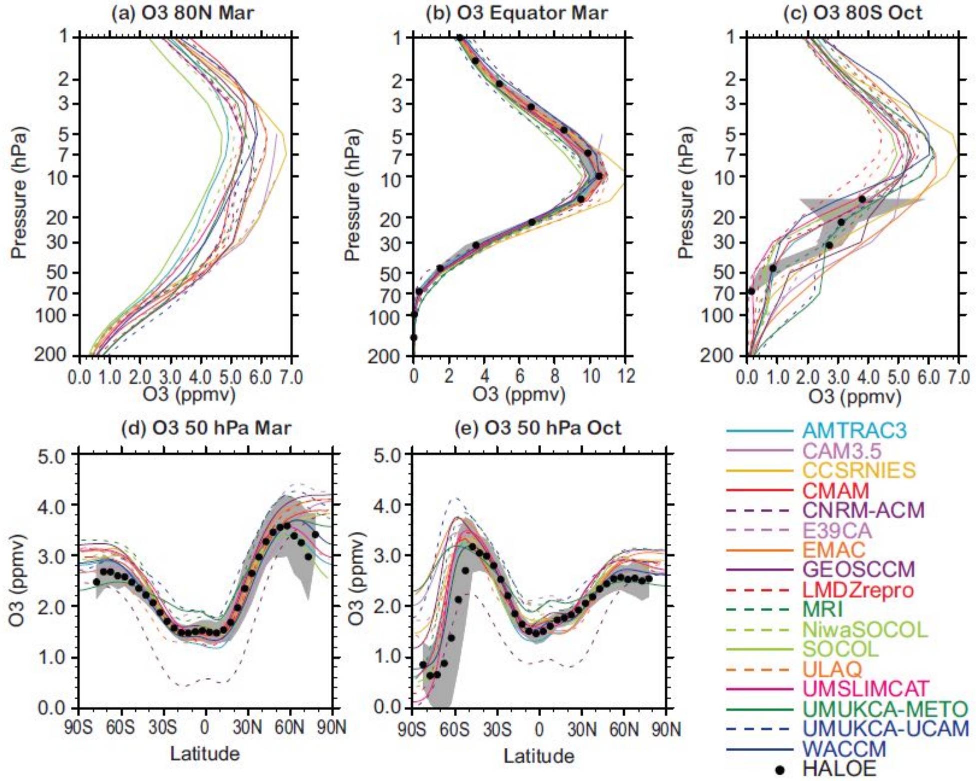


Figure 3: Climatological zonal mean ozone mixing ratios from CCMs and HALOE (in ppmv). Vertical profiles at (a) 80°N in March, (b) Equator in March, and (c) 80°S in October. Latitudinal profiles at 50 hPa in (d) March and (e) October. The grey area shows HALOE ±1 standard deviation (s) about the climatological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

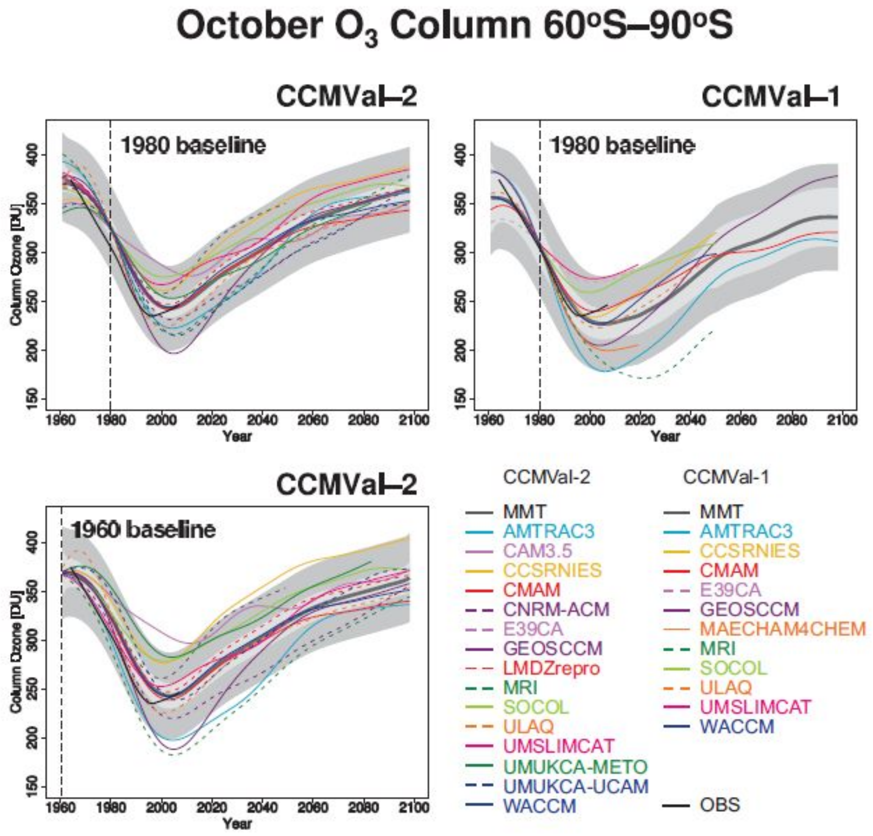
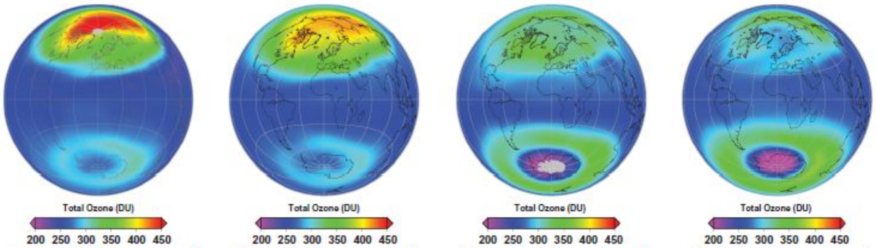
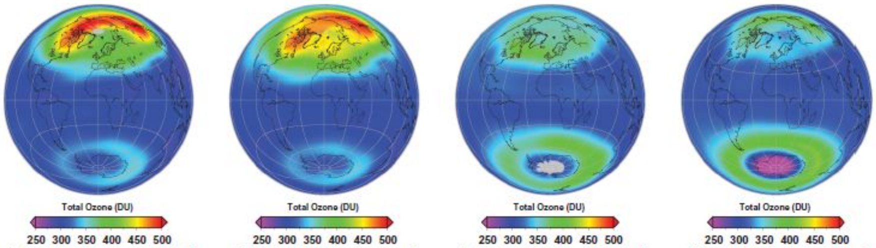


Figure 4: 1980 baseline-adjusted multi-model trend (MMT) estimates of annually averaged total ozone for the latitude range 60°S-90°S for the month of October (heavy dark grey line) with 95% confidence and 95% prediction intervals appearing as light- and dark-grey shaded regions about the trend (upper 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 from SPARC CCMVal, 2010.)

Figure 5 gives a nice example for a future oriented comparison of observations and CCM results. It is based on climatological mean values which needs long-term, consolidated data series. The data basis of observations are measurements from the three satellite borne instruments: For the first time global total ozone columns from the European satellite sensors GOME (ERS-2), SCIAMACHY (ENVISAT), and GOME-2 (METOP-A) are combined and added up to a continuous time series starting in June 1995 (Loyola et al., 2009).



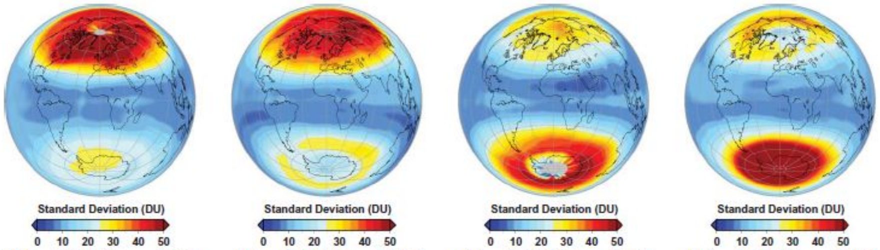
(a) Satellite total ozone winter (DJF)
(b) Satellite total ozone spring (MAM)
(c) Satellite total ozone summer (JJA)
(d) Satellite total ozone autumn (SON)



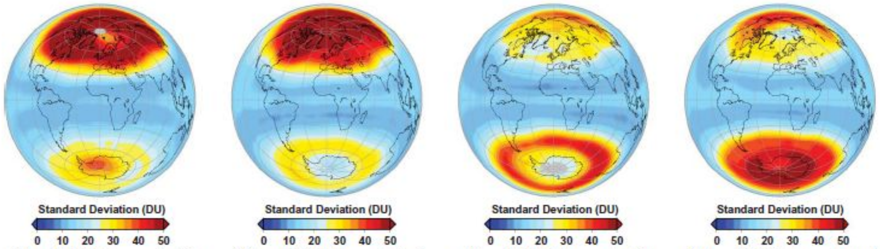
(e) E39C-A total ozone winter (DJF)
(f) E39C-A total ozone spring (MAM)
(g) E39C-A total ozone summer (JJA)
(h) E39C-A total ozone autumn (SON)

Figure 5: Seasonal mean values of total ozone (June 1995 to May 2008, in Dobson Units, DU) from satellite instruments GOME, SCIAMACHY, and GOME-2 (top) and a respective simulation of the CCM E39C-A (bottom). (Figure 9 from 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 basement 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.



(a) Satellite total ozone standard dev. winter (DJF)
(b) Satellite total ozone standard dev. spring (MAM)
(c) Satellite total ozone standard dev. summer (JJA)
(d) Satellite total ozone standard dev. autumn (SON)



(e) E39C-A total ozone standard dev. winter (DJF)
(f) E39C-A total ozone standard dev. spring (MAM)
(g) E39C-A total ozone standard dev. summer (JJA)
(h) E39C-A total ozone standard dev. autumn (SON)

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 from Loyola et al., 2009.)

Figure 7 illustrates another conventionally 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 fluctuation 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.

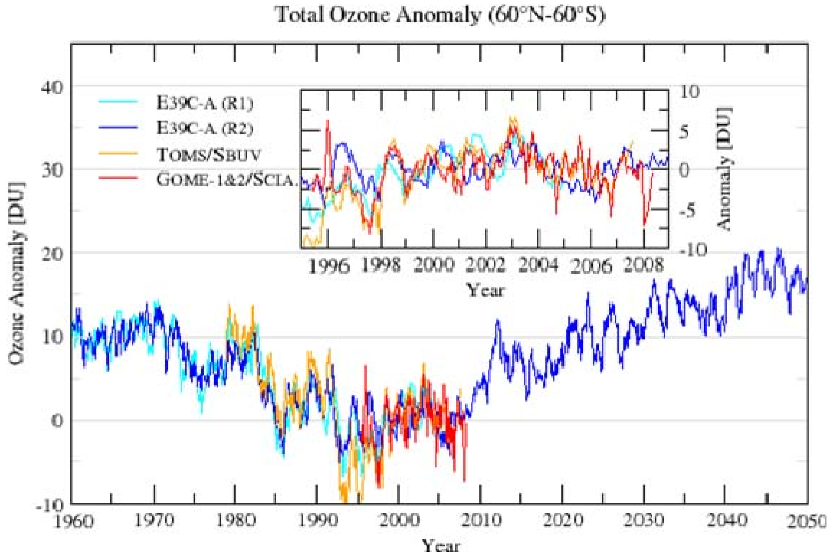


Figure 7: Total ozone anomalies over 60°N to 60°S. The mean annual cycle for 1995 to 2004 is subtracted from satellite measurements (orange and red) and two E39C-A model simulations R1 from 1960 to 2004 (cyan) and R2 from 1960 to 2050 (blue). The inset shows a close-up for years where satellite measurements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

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.

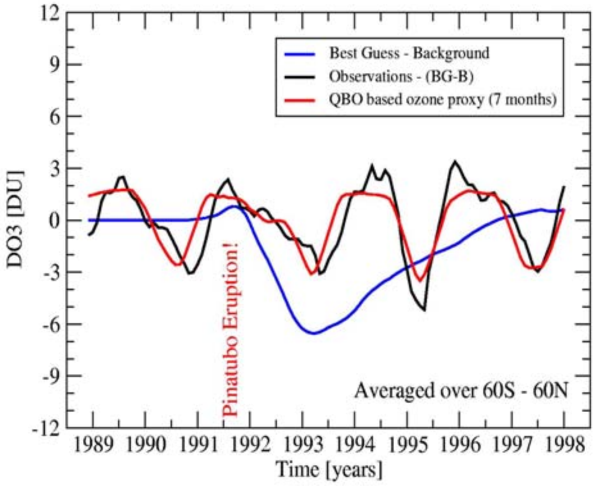


Figure 8: Time series of global ozone anomalies. Blue: ozone change due to volcanic aerosol; Black: residual ozone change; Red: a QBO based ozone proxy. Note the good agreement between the black and red line.

As mentioned, these examples are shown to demonstrate how evaluation of model results (here in particular 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 will be created in the Ozone_cci project, i.e. merged regridded, multi-sensor data sets covering long-term (multi-year) periods, will represent a significant additional value to recently available data products because they will obviously reduce the above mentioned inadequatenesses.

6 Product requirements and traceability

6.1 Introduction

ECV data sets produced within the ozone_cci project fall into two categories, a column integrated product (total ozone) and two vertically resolved products (limb and nadir sounded ozone profiles). 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 68% 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 68% 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.

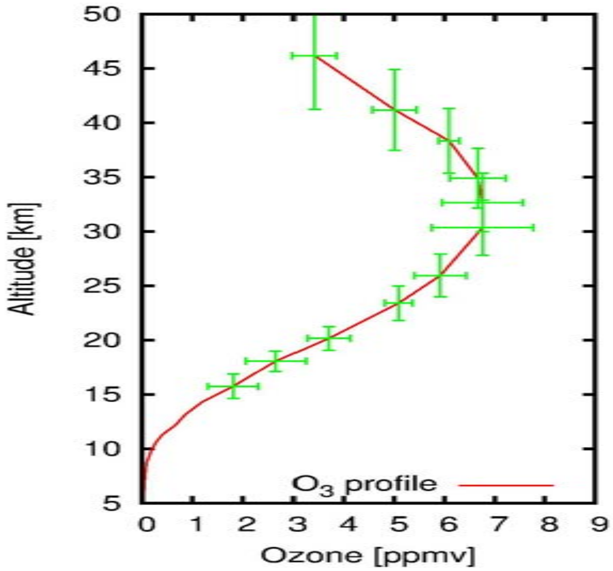


Figure 9: Sketch illustrating an ozone profile and the reporting of errors.

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 build 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 providing e.g. 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 will distinguish between research topics and will 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.

In contrast to GCOS canonical requirements, which are mainly justified on the commonly used standard resolution of currently available and used model systems, the requirements defined in Ozone_cci are linked to driving research topics of relevance for our Climate Research Group. These follow on the scientific rationale defined in section 4.

6.2 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 UNEP/WMO Scientific Assessment of Ozone Depletion: 2010, 2011). 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 (in 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 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 lowest accuracy over the targeted time period.

The required precision is always the same as for the tabulated accuracies under the assumption that the important biases in the products will be fully characterized.

Table 5: Requirements for total ozone. Achievable and future target requirements are given, separated by a '–'.

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*	3 days	3 days	3 days
Time period	Evolution of the ozone layer (radiative forcing)	(1980-2010)	(1980-2010)	(1980-2010)
Accuracy	Evolution of the ozone layer (radiative forcing)	2% (7 DU)	2% (7 DU)	2% (7 DU)
Accuracy	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 (1980-2010 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 6: Data requirements for total ozone

Data feature	**Requirement**
Data format	netCDF
Data conventions	CF
Error	Total area
Error characteristics (optional)	Total accuracy 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)

6.3 Ozone profile data product from nadir-viewing instruments

As for 6.2 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 a coarser vertical resolution is acceptable (~6 km) also because these 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 minimum targeted time period for the nadir ozone profiles covers 15 years (1996-2010). 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 lowest accuracy over the targeted time period.

The required precision is always the same as for the tabulated accuracies under the assumption that the important biases in the products will be fully characterized.

Table 7: Product requirements for nadir-based ozone profiles. 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 25 km, and the middle atmosphere extends from about 25 to 60 km altitude. The required coverage is global. Achievable and future target requirements are given, separated by a '–'.

Quantity	**Driving Research topic**	**Height range**		
		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	20 – 200 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	3 – 6 km	3 – 10 km
Observation frequency	Evolution of the ozone layer and the tropospheric ozone burden (radiative forcing); Seasonal cycle and interannual variability; Short-term variability*	3 days	3 days	3 days
Time period	Evolution of the ozone layer and tropospheric ozone burden (radiative forcing)	(1980-2010) – (1996-2010)	(1980-2010) – (1996-2010)	(1980-2010) – (1996-2010)
Accuracy	Evolution of the ozone layer and tropospheric ozone burden (radiative forcing)	10 %	8 %	8 %
Accuracy	Seasonal cycle and interannual variability; Short-term variability*	20 %	15 %	15 %
Stability	Evolution of the ozone layer and tropospheric ozone burden (radiative forcing); trends	1 – 3 % / decade	1 – 3 % / decade	1 – 3 % / decade

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

Table 8: Data requirements for nadir-based ozone profiles

Data feature	**Requirement**
Data format	netCDF
Data conventions	CF
Error characteristics	Total accuracy 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)

6.4 Ozone profile data product from limb-viewing instruments

As for 6.2 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 from 2003 onward (2003-2010), although for climate research longer term records would be desirable. 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.

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 always the same as for the tabulated accuracies under the assumption that the important biases in the products will be fully characterized.

Table 9: Product requirements for limb-based ozone profile requirements. . The lower stratosphere (LS) extends from the tropopause (defined as ozone > 150 ppbv) to about 25 km, and the middle atmosphere extends from about 25 to 60 km altitude. The required coverage is global.

Quantity	**Driving Research topic**	**Height Range**	
		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 – 300 km	100 – 300 km
Vertical resolution	Height dependence of evolution of the ozone layer (radiative forcing); Seasonal cycle and interannual variability; Short-term variability*	1 – 3 km	3 – 5 km
Observation frequency	Seasonal cycle and interannual variability; short-term variability*	3 days	3 days
Time period	Evolution of the ozone layer (radiative forcing)	(1980-2010) – (2003-2010)	(1980-2010) – (2003-2010)
Accuracy in height attribution	Evolution of the ozone layer(radiative forcing), Seasonal cycle and interannual variability; Short-term variability*	±500 m	±500 m
Accuracy for mixing ratio	Evolution of the ozone layer (radiative forcing)	8%	8%
Accuracy for mixing ratio	Seasonal cycle and interannual variability; Short-term variability*	15 %	15 %
Stability	Evolution of the ozone layer (radiative forcing); trends	1 – 3 % / decade	1 – 3 % / decade

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

Table 10: Data requirements for limb-based ozone profile requirements

Data feature	**Requirement**
Data format	NetCDF
Data conventions	CF
Error characteristics	Total accuracy 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)

6.5 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.

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