



TITLE:

## Ozone\_cci phase II



### Product Specification Document (PSD)

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Phase 2

**WP Manager:** R.J. van der A

**WP Manager Organization:** KNMI

**Other partners:**

**CRG:** DLR-PA , KIT, KNMI

**EOST:** DLR-IMF, BIRA-IASB, KNMI, RAL, IUP-Bremen, LATMOS, ULB,  
U.SASK, CHALMERS, UofT



## DOCUMENT CHANGE RECORD

Issue	Revision	Date	Modified items
0	4	08/04/2011	Draft version submitted to CMUG and ESA for comments
1	0	12/04/2011	<ul style="list-style-type: none"><li>- requirement tables removed, and text generally reorganised to avoid any duplication with the URD. The PSD now includes (1) a brief description of the model tools specific to the project, (2) a definition of the ozone_cci products and of their usefulness for climate-related studies, and (3) a detailed specification of the data products</li><li>- data product specification tables added for columns, nadir profiles and limb profiles</li><li>- cross-reference to URD tables given as appropriate</li></ul>
1	1	29/04/2011	Final version approved by ESA
2	0	29/06/2011	Revised version according to preliminary remarks from CMUG
2	1	1/07/2011	Time period specifications clarified and added to Table 1
3	0	15/12/2011	<p>Following changes have been introduced, in response to remarks and suggestions from CMUG:</p> <ul style="list-style-type: none"><li>- simplified introduction</li><li>- revised product overview section → includes time lines for data products to be generated in both phases of the CCI</li><li>- revised product specification sections → includes new introductory parts, new tables summarizing target systematic and random uncertainties for the data products, simplified product specification tables; data format specification for both level-2 and level-3 data where relevant</li></ul>
3	1	04/04/12	Change accuracy/precision by systematic/random uncertainties
4	0	28/07/14	Starting point for phase 2
4	2	15/08/14	Updates included from Chalmers, Univ. Toronto, FMI, KNMI, RAL, ULB, BIRA-IASB
4	3	22/09/14	Updates of Table 1 and section 6.
4	4	02/10/14	Update of IASI format Table in section 6.
4	5	02/10/14	Minor updates in total ozone specifications
4	6	03/11/15	Updates from BIRA-IASB, ULB and KNMI



			Including of tropospheric ozone products
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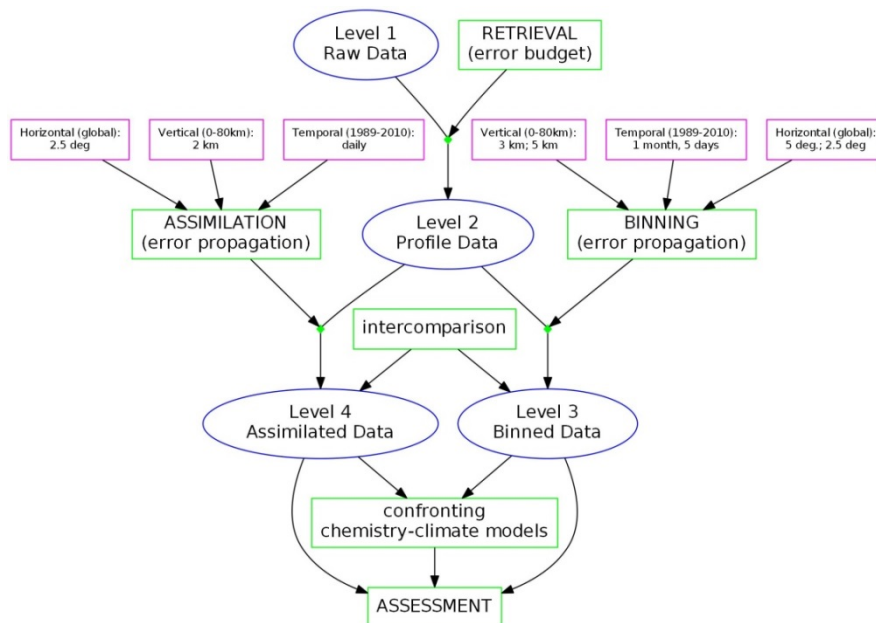
# 1 Introduction

The purpose of the product specification document (PSD) is to provide detailed specifications for the ozone Essential Climate Variable (ECV) data products that will be generated within the second phase of the Ozone\_cci project. It will outline the product specifications for each level-2, level-3 and level-4 data product that will be generated in the second phase of the CCI. These specifications will be compliant with the wishes from the climate user community as specified in the User Requirement Document (URD).

The ECV data products belong to three main families as defined in the ESA SOW:

- total column data products,
- vertical profiles derived from nadir viewing instruments
- vertical profiles derived from limb and occultation sensors.

The primary objective of the Ozone\_cci project is to develop new and improved methods to generate long-term high-quality ozone data products from ESA and ESA Third Party Mission sensors. In terms of product generation, efforts concentrate on (1) improving and homogenizing current level-2 ozone column and profile data sets from nadir UV sensors; (2) designing data merging techniques suitable to create blended multi-sensor data sets (level-3 and level-4) for the three types of Ozone\_cci ECV data products.



**Figure 1:** Flowchart showing the logic of the data product development and usage in the Ozone\_cci project, starting from level 1 to level 4 data sets. The diagram is primarily for vertical profile data developed from nadir and limb-viewing sensors. Total ozone is a special case where level-2 data become more directly level-3, but binning and assimilation happens similarly as well.



Figure 1 graphically describes the logic of the data product development and their usage in the Ozone\_cci project, starting from radiance measurements (level 1) down to assimilated data sets (level 4). Note that although the flowchart is primarily valid for vertical profile data developed from nadir and limb-viewing sensors, total ozone can be considered as a special case where level-2 data become more directly level-3 without consideration of the vertical axis. Binning and assimilation happens similarly as for other data products.

This product specification document builds upon the User Requirement Document (URD). Overall, the aim of the ESA Climate Change Initiative is to develop ECV products that meet the needs of the Global Climate Observing System (GCOS). Although algorithm developments and data characterisation work to be performed in Ozone\_cci will lead to significant progress towards meeting the climate user requirements, it must be noted that mature data products do not necessarily exist yet. The purpose of the present document is to outline the current product specifications for each data product with the understanding that this specification may be incomplete and/or is expected to change in the course of the project.

In Section 2, the different ozone instruments used in the project are briefly introduced. Section 3 presents an overview of the various level-2, level-3 and level-4 data products that will be generated in the current phase of the CCI. Detailed specifications are then provided for total ozone, nadir ozone profile and limb ozone profiles respectively in Sections 5, 6 and 7. This includes in particular a description of the NetCDF Climate and Forecast (CF) convention that will be systematically used for level-3 data reporting in agreement with requirements expressed by the climate user community.



## 2 Instruments

Ozone can be measured by a variety of sensors and measurements techniques. In this project, we focus more particularly on ESA and ESA Third Party Mission (ESA-TPM) sensors from which three distinct lines of ozone data products are derived: total ozone, ozone profiles at low vertical resolution from nadir sensors and ozone profiles at high vertical resolution in the stratosphere and UT/LS from limb-type sensors.

### 2.1 Nadir-type sensors

#### 2.1.1 GOME/ERS-2

The GOME (Global Ozone Monitoring Experiment) instrument is a 4 channel UV/Vis grating spectrometer observing the earth's atmosphere in nadir viewing geometry. It has a moderate spectral resolution of 0.2 - 0.4 nm and a ground-pixel size of 320 x 40 km<sup>2</sup> (960 x 40 km<sup>2</sup> for the back scan). A detailed description of the instrument is given in Burrows et al. (1999). GOME was launched on ERS-2 into a sun synchronous polar orbit in April 1995, and has been delivering data until June 2011 when the ERS-2 platform was shut down. However as a result of aging problems of the ERS-2 platform, pointing accuracy is reduced since February 2001. This affects mainly the solar measurements of GOME, decreasing the frequency of good solar irradiance measurements and thereby increasing noise in some products. Further, since June 2003, a permanent failure of the last tape recorder on ERS-2 limits GOME coverage to areas where direct downlink of data is possible. In Ozone\_cci, GOME measurements are used to retrieve total columns and vertical distributions of ozone. Because of its proven stability and of its long lifetime (16 years), GOME is generally considered as the European “Gold Standard” for total ozone measurements.

#### 2.1.2 GOME-2/METOP

GOME-2 is on-board the EUMETSAT satellite MetOp-A which was launched in October 2006. Build on a design almost identical to GOME, it covers the same spectral range as its predecessor but with an improved spatial resolution. The nominal ground-pixel size is 80 x 40 km<sup>2</sup> with a global coverage in almost one day (swath of 1920 km). GOME-2 continues the measurement series started with GOME, and in this project it is therefore used to retrieve total columns and vertical distributions of ozone. Data are available since January 2007 on an operational basis. A second GOME-2 instrument has been launched in 2012 on the METOP-B platform, and a third one will be launched at the end of the decade on METOP-C.

#### 2.1.3 OMI/AURA

The Ozone Monitoring Instrument (OMI) is a nadir viewing imaging spectrograph that measures the solar radiation backscattered by the Earth's atmosphere and surface over the entire wavelength range from 270 to 500 nm with a spectral resolution of about 0.5 nm. OMI was launched on-board the NASA satellite AURA in July 2004. In comparison to the GOME and SCIAMACHY sensors, OMI is characterized by a larger swath width of 2600 km, which enables measurements with a daily global coverage at all latitudes. The nominal OMI pixel size of 13 ×



24 km<sup>2</sup> at nadir is also significantly smaller. The small pixel size enables OMI to look in between the clouds, which is important for retrieving tropospheric information. The light entering the telescope is also depolarised using a scrambler, which avoids polarization-related artefacts. OMI data are available since 2004 and the instrument is still operational, however in 2007 OMI started to experience the so-called row anomaly which reduces the amount of useful measurements, despite correction algorithms being implemented in the level-1 processing chain. In the project, the OMI instrument is used for ozone profile retrievals. OMI total ozone data are also used for intercomparison and validation with total ozone data products developed from the GOME, SCIAMACHY and GOME-2 sensors.

#### **2.1.4 SCIAMACHY/ENVISAT**

SCIAMACHY (Scanning Imaging Absorption Spectrometer for Atmospheric CHartography) is a multi-channel UV-Vis-NIR spectrometer launched on the ENVISAT platform in 2002. Its primary mission objective is the global monitoring of trace gases in the troposphere and in the stratosphere. The solar radiation transmitted, backscattered and reflected from the atmosphere is recorded at medium resolution (0.2 nm to 1.5 nm) over the range 240 nm to 1700 nm, and in selected regions between 2.0 µm and 2.4 µm. SCIAMACHY is particular since it has three different viewing geometries: nadir, limb, and sun/moon occultation, which yield total column values as well as distribution profiles in the stratosphere and upper troposphere. In this project both nadir and limb measurements are used in Channels 1, 2 and 3. In nadir view, used for ozone total column and vertical profile retrievals, the ground pixel size for channels 2-3 is 30x60 km<sup>2</sup>, i.e. a resolution intermediate between GOME and OMI. The swath width of SCIAMACHY at nadir is similar to GOME (960 km), however due to the alternate nadir and limb mode operation, global coverage is only obtained in approximately 6 days. In limb view, ozone number density profiles are derived in the stratosphere by exploiting the Hartley and Chappuis spectral absorption bands in channels 1 and 3. SCIAMACHY data are available from July 2002 till April 2012 when communication with ENVISAT was lost.

#### **2.1.5 IASI/METOP**

The Infrared Atmospheric Sounding Interferometer (IASI) is nadir looking Fourier Transform Spectrometer associated with an imaging instrument launched on the METOP series of European meteorological EUMETSAT's polar-orbit satellites. The mission is dedicated to high-resolution atmospheric sounding of trace gases like ozone, methane or carbon monoxide on a global scale and to operational meteorological soundings with a high accuracy requirement (1 K for tropospheric temperature and 10% for humidity with a vertical resolution of 1 km). Two IASI instruments have been successively launched in October 2006 and in September 2012 on MetOp-A and -B. A third instrument will be launched on MetOp-C satellite and will continue to operate until 2020. The METOP satellites are sun-synchronous with a 98.7° inclination to the equator, and a global coverage twice daily at about 09:30 and 21:30 local time. Each of the two launched MetOp platforms makes a little more than 14 orbits a day. IASI is a cross-track scanner covering the infrared spectral domain from 645 to 2,760 cm<sup>-1</sup> (3.62–15.5 µm) with a total of 30 ground fields of regard (FOR) per scan. The spectrum is measured in three wavelength bands (8.26–15.5, 5.0–8.26, and 3.62–5.0 µm), with a separate detector allowing the continuous spectral coverage with no gaps, and each FOR measures a 2x2 array of footprints characterized by a 12-





km diameter at nadir. The apodized spectral resolution is  $0.5 \text{ cm}^{-1}$  and each spectrum is sampled every  $0.25 \text{ cm}^{-1}$  providing a total of 8461 radiance channels.

## **2.2 Limb and occultation type sensors**

### **2.2.1 MIPAS/ENVISAT**

MIPAS (Michelson Interferometer for Passive Atmospheric Sounding) is an infrared limb emission sounder on ENVISAT, designed and operated for measurements of constituents between the upper troposphere and the mesosphere. MIPAS is a rear looking instrument with the lines of sight approximately in the orbit plane. In the original measurement mode, which was operational from July 2002 to March 2004, 17 tangent altitudes between 6 and 68 km were measured per limb scan at a spectral resolution of  $0.035 \text{ cm}^{-1}$  (unapodized). However since January 2005, due to a mirror failure, MIPAS is operating on reduced spectral resolution mode ( $0.0625 \text{ cm}^{-1}$ ). MIPAS measures ozone vertical profiles day and night on the altitude range from 6 to 70 km, pole-to-pole. Data are available for July 2002-March 2004 and January 2005 until April 2012 when communication with ENVISAT was lost. Global coverage is obtained in approximately 3 days.

### **2.2.2 GOMOS/ENVISAT**

GOMOS (Global Ozone Monitoring by Occultation of Stars) is a medium resolution spectrometer covering the wavelength range from 250 nm to 950 nm. It measures attenuation of stellar light in occultation geometry. From dark-limb occultations in the UV-Visible and IR spectral ranges, the vertical profiles of ozone are retrieved in the altitude region from 15 to 100 km. In comparison to other limb-type sensors on ENVISAT, GOMOS features a high vertical resolution of the retrieved ozone profiles is 2 km below 30 km, 3 km above 40 km, with a linear growth from 2 km to 3 km in the altitude range 30-40 km. However the quality of the retrieved profiles can depend on the type of star used as a source as well as on the geometry of the occultation (the latter due to the scintillation phenomenon). Careful selection and error characterization are necessary to make best use of the data products. GOMOS data are available from 2002 till 2012. Summer poles are not covered, due to the absence of night-time conditions. Data from May-June 2003, January-July 2005 and February-November 2009 are not available due to the instrument technical anomalies.

### **2.2.3 SCIAMACHY/ENVISAT**

See Section 2.1.4

### **2.2.4 OSIRIS**

OSIRIS (Optical Spectrograph and InfraRed Imaging System) is a Canadian instrument on board the Swedish satellite Odin that was launched in February of 2001. It is a limb-viewing device that makes repeated measurements of the limb scattered radiance with a sampling of



approximately 2 km between 10 km and 100 km of altitude. OSIRIS is used to generate ozone profiles in a range from 80° S to 80° N. Concentrations are retrieved on a 1 km grid from 10.5 km to 59.5 km, using a retrieval approach similar in concept to the one used for SCIAMACHY in its limb mode. The OSIRIS instrument is still operational.

### **2.2.5 SMR**

The Sub-Millimetre Radiometer (SMR) onboard the Odin satellite, has been launched in February 2001. Measurements of thermal emission lines are performed during day and night and global coverage is achieved during one observation day. Vertical profiles of ozone and many other species are retrieved using retrieval algorithms based on the Optimal Estimation Method. The official operational level-2 data are produced by the Chalmers University of Technology in Göteborg, Sweden. In this project, we use the currently recommended version 2.1 ozone data product that provides stratospheric ozone data in the ~12-50km range with 2.5-3.5km vertical resolution and single-profile precision of about 20%. The Odin data set is available from November 2001 until present.

### **2.2.6 ACE-FTS**

ACE-FTS is on-board the Canadian satellite SCISAT launched in August 2003, and data is available from Feb. 2004 to present. It provides latitudinal coverage from about 85°N to 85°S with complete coverage every 3 months. In this project, we use the ACE-FTS level-2 data products that are generated at the ACE Science Operations Centre at the University of Waterloo. The ACE-FTS is a high-resolution ( $0.02 \text{ cm}^{-1}$ ) Fourier transform spectrometer measuring from 2.2 to  $13 \mu\text{m}$  ( $750 - 4400 \text{ cm}^{-1}$ ). Operating in solar occultation mode, the ACE-FTS provides detailed profiles of the Earth's atmosphere for more than 30 chemical species. The altitude range of the retrieved ozone profiles is from cloud tops (~5 km) to 95 km and the vertical resolution is ~3-4 km (based on the field-of-view of the ACE-FTS instrument).



### 3 Products overview

This section presents an overview of the different data products that will be generated in the project. Detailed specifications are given in the next sections.

Although the primary Ozone\_cci end products are multi-sensor merged data sets, i.e. level-3 and level-4 data, several intermediate level-2 data sets will also be produced as an input for the multi-sensor data sets. We distinguish between level 3 or level 4 data depending whether they result from simple binning of observations only, or from model-based assimilation tools. Tables 1a, 1b and 1c list all the data sets that are planned to be delivered in the second phase of the CCI programme.

Data products are identified according to the following convention:

PRD\_LV\_INST\_PRO

where:

- PRD is the product, i.e. ‘TC’, ‘NP’, ‘LP’, ‘UTLS’, ‘MLT’ and ‘TROPOL’ for ozone total column, ozone nadir profiles, ozone limb profiles, upper-troposphere-lower-stratosphere ozone, Mesosphere-Lower-Thermosphere ozone and tropospheric ozone column respectively;
- LV is the product level, i.e. ‘L2’, ‘L3’, ‘L4’;
- INST is the instrument, for multi-sensor merged or assimilated products use ‘MRG’;
- PRO is the processing centre;

#### *Comment on data formatting*

Note that all level 3 products that will be generated in the project will be designed to be compliant with NetCDF Climate and Forecast (CF) convention for the data structure and with the INSPIRE standard for the metadata.

NetCDF-CF version 1.4 is used with metadata attributes following the NetCDF-CF naming convention (<http://cf-pcmdi.llnl.gov/documents/cf-standard-names/>).



**Table 1a.** Overview of the Level 2 data products to be generated and delivered in Ozone\_cci CRDP Final (European sensors only). The data sets already delivered/processed at the end of Phase-I are represented in dark green. We assume that the currently available sensors will still be in operation by the end of 2015.

L2 Data Product	Processing entity	Time period																				
			96	97	98	99	00	01	02	03	04	05	06	07	08	09	10	11	12	13	14	15
TC_GOME	BIRA		Dark Green	Dark Green	Dark Green	Dark Green	Dark Green	Dark Green	Dark Green	Dark Green	Dark Green	Dark Green	Dark Green	Dark Green	Dark Green	Dark Green	Dark Green	Dark Green	Dark Green	Dark Green	Dark Green	Dark Green
TC_SCIAMACHY	BIRA								Dark Green	Dark Green	Dark Green	Dark Green	Dark Green	Dark Green	Dark Green	Dark Green	Dark Green	Dark Green	Dark Green	Dark Green	Dark Green	Dark Green
TC_GOME2A	BIRA														Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green
TC_GOME2B	BIRA																		Light Green	Light Green	Light Green	Light Green
TC_OMI	BIRA									Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green
TC_OMPS#	BIRA																		Light Green	Light Green	Light Green	Light Green
NP_GOME	RAL		Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green
NP_SCIAMACHY	RAL								Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green
NP_GOME2A	RAL												Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green
NP_GOME2B	RAL																		Light Green	Light Green	Light Green	Light Green
NP_OMI#	RAL									Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green
NP_IASI	ULB														Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green
LP_SCIAMACHY	UBR/FMI								Dark Green	Dark Green	Dark Green	Dark Green	Dark Green	Dark Green	Dark Green	Dark Green	Dark Green	Dark Green	Dark Green	Dark Green	Dark Green	Dark Green
LP_OMPS#	UBR/FMI																		Light Green	Light Green	Light Green	Light Green
LP_MIPAS	KIT/FMI								Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green
LP_GOMOS	ESA/FMI								Dark Green	Dark Green	Dark Green	Dark Green	Dark Green	Dark Green	Dark Green	Dark Green	Dark Green	Dark Green	Dark Green	Dark Green	Dark Green	Dark Green
LP_OSIRIS	UoS/FMI								Dark Green	Dark Green	Dark Green	Dark Green	Dark Green	Dark Green	Dark Green	Dark Green	Dark Green	Dark Green	Dark Green	Dark Green	Dark Green	Dark Green
LP_SMR	CHALM/FMI								Dark Green	Dark Green	Dark Green	Dark Green	Dark Green	Dark Green	Dark Green	Dark Green	Dark Green	Dark Green	Dark Green	Dark Green	Dark Green	Dark Green
LP_ACE	UoT/FMI											Dark Green	Dark Green	Dark Green	Dark Green	Dark Green	Dark Green	Dark Green	Dark Green	Dark Green	Dark Green	Dark Green
LP_SAGEII	FMI	84-	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green
LP_HALOE	FMI	91-	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green
UTLS_SCIA	UBR/FMI									Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green
UTLS_MIPAS	KIT/FMI									Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green
UTLS_GOMOS	FMI									Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green
UTLS_OSIRIS	UoS/FMI								Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green
UTLS_ACE	UoT/FMI											Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green
MLT_MIPAS_DN_DCA*	KIT																					
MLT_GOMOS_DN_DCA*	ESA/KIT									Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green
MLT_ACE_DN_DCA*	UoT/KIT											Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green
MLT_SMR_DN_DCA*	CHALM/KIT								Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green
MLT_MIPAS_SM#	KIT/IAA											Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green	Light Green

- TC Total Column product
- NP Nadir Profile product
- LP Limb Profile product
- UTLS Upper Troposphere and Lower Stratosphere product
- MLT Mesosphere and Lower Thermosphere product
- DN Day and Night separated
- SS Sunrise and Sunset separated



DCA Diurnal Correction Applied  
SM Special Mode (MIPAS mode optimised for the mesosphere)  
\* Only if development of a diurnal correction scheme is successful  
# Proposed as an option



Table 1b: Overview of the Level 3 and 4 data products to be delivered in Ozone\_cci CRDP Final (European sensors only). The data sets already delivered/processed at the end of Phase-I are represented in dark green. We assume that the currently available sensors will still be in operation by the end of 2015.

L3/4 Data Product	Processing entity	Time period																				
			96	97	98	99	00	01	02	03	04	05	06	07	08	09	10	11	12	13	14	15
TC_MRG	DLR		█	█	█	█	█	█	█	█	█	█	█	█	█	█	█	█	█	█	█	█
NP_MRG	KNMI		█	█	█	█	█	█	█	█	█	█	█	█	█	█	█	█	█	█	█	█
NP_ASSIM	KNMI		█	█	█	█	█	█	█	█	█	█	█	█	█	█	█	█	█	█	█	█
TTOC_GOME	DLR		█	█	█	█	█	█	█	█	█	█	█	█	█	█	█	█	█	█	█	█
TTOC_GOME2A <sup>∞</sup>	DLR																					
TTOC_GOME2B <sup>∞</sup>	DLR																					
LNTOC_ENVISAT	UBR																					
LNTOC_OMPS	UBR																					
LNTOC_OMPSG2#	UBR																					
LP_SCIA_MZM	UBR/FMI																					
LP_OMPS_MZM#	UBR/FMI																					
LP_MIPAS_MZM	KIT/FMI																					
LP_GOMOS_MZM	ESA/FMI																					
LP_OSIRIS_MZM	UoS/FMI																					
LP_SMR_MZM	CHALM/FMI																					
LP_ACE_MZM	UoT/FMI																					
LP_SAGEII_MZM	FMI	84-	█	█	█	█	█	█	█	█	█	█	█	█	█	█	█	█	█	█	█	█
LP_HALOE_MZM	FMI	91-	█	█	█	█	█	█	█	█	█	█	█	█	█	█	█	█	█	█	█	█
LP_MRG_MZM	FMI																					
LP_MRG_BWM	FMI																					
LP_MRG_FRM	FMI																					
UTLS_SCIA_L3\$	UBR/FMI																					
UTLS_MIPAS_L3\$	KIT/FMI																					
UTLS_GOMOS_L3\$	FMI																					
UTLS_OSIRIS_L3\$	UoS/FMI																					
UTLS_ACE_L3\$	UoT/FMI																					
UTLS_MRG_L3\$	FMI																					
MLT_MIPAS_MZM_DN	KIT/IAA																					
MLT_MIPAS_MZM_DN_DCA*	KIT/IAA																					
MLT_MRG_MZM_DN	KIT/IAA																					
MLT_MRG_MZM_DCA*	KIT/IAA																					

- TC Total Column product
- NP Nadir Profile product
- LP Limb Profile product
- UTLS Upper Troposphere and Lower Stratosphere product
- MLT Mesosphere and Lower Thermosphere product
- MRG Merged data set
- ASSIM Assimilated data set
- TTOC Tropical Tropospheric Ozone Column





## 4 File naming convention

The proposed generic filename convention is as follows:

CCI\_O3\_PRD\_INST\_LV\_YYYYMMDD\_ddd\_PRO\_RV.TYPE

where

- PRD is the product, i.e. ‘TC’, ‘NP’, ‘LP’ for ozone total column, ozone nadir profiles and ozone limb profiles respectively;
- INST is the sensor name, e.g. ‘MIPAS’, ‘SCIAMACHY’, etc. In the case of merged data products generated from the combination of several sensors, the specification is ‘MRG’
- LV is the product level, i.e. ‘L2’, ‘L3’, ‘L4’;
- YYYYMMDD is the sensing start year, month and day;
- ddd is duration of the product, i.e. ‘Ddd’ for dd days, ‘Wdd’ for dd weeks, ‘Mdd’ for dd months, ‘Ydd’ for dd years;
- PRO is the processing centre;
- RV is the two digit product revision; and
- TYPE denotes the product format used, i.e. ‘nc’ for netCDF.

In the same way we can use the following directory structure for disseminating the products (e.g. via FTP):

PRD/SENSOR/LV/YYYY/MM/DD

As implied above, two *product* types will be produced: total ozone in Dobson Units [DU] and ozone volume mixing ratios [ppmv]. The *product* type specifiers can be total, limb or nadir. Total ozone shall be abbreviated **toz** and ozone volume mixing ratio **ozvmr**. Long names should reflect the CF convention: “atmosphere mass content of ozone” for toz; “mole fraction of ozone in air” for ozvmr. The short names will be allowed to vary for legacy reasons but the use of toz and ozvmr are encouraged.

More options for the file naming convention can be found in Guidelines for Data Producers.





## 5 Total ozone data products

Total ozone data sets covering different time periods have been derived from different instruments (e.g. TOMS, OMI, GOME, SCIAMACHY, etc). For climatological assessments and investigations of long-term changes individual instrument records are mostly too short and it is necessary to merge data sets available on shorter periods from different instruments. One fundamental problem is that the recent total ozone data sets (in particular from ESA and ESA TPM sensors) are currently not consistently harmonised and therefore do not provide a solid basement for robust analyses of short- and long-term fluctuations. To cope with this issue, fall back approaches have been recently used that rely on empirical corrections applied to individual data sets to compensate for inconsistencies. Such approaches however have limitations that make reliable scientific conclusions difficult. In particular the range of uncertainty of such data products is often unknown or undefined.

In the Ozone\_cci phase-I project, we have made a significant progress towards harmonisation of the European total ozone data set by using a common state-of-the-art algorithm for the different instruments GOME, SCIAMACHY and GOME-2. The quality of the level-2 data products has been significantly improved through systematic implementation of the GOME-type direct-fitting retrieval scheme (GODFIT) developed at BIRA-IASB in close cooperation with DLR and RT-Solutions. This algorithm is based on a least-squares fitting including direct multi-spectral radiative transfer simulation of radiances and retrieval parameters Jacobians. In addition, to minimize the impact of instrument-specific level-1 errors, reflectance corrections determined using vicarious calibrations at reference sites have been applied. The data from the newly developed level-2 retrieval algorithm has been then combined in level-3 data products covering the full period from 1995 until 2011. During the phase-II of the Ozone\_cci project, the L1 data sets from OMI/Aura, GOME-2/Metop-B and OMPS will be fully reprocessed with the same algorithm in order to further extend the ESA CCI total ozone climate data records. Additionally, new algorithmic developments will be carried out in order to further enhance the product quality and also to improve the consistency with the ozone nadir profile ECV data records.

In the following, the target uncertainties and product specifications tables for level 2 and level 3 total ozone data products are presented. All total ozone data products generated in Ozone\_cci will follow the user requirements for NetCDF CF standard.

### 5.1 Target uncertainties for CCI total ozone data products

Quantity	
Horizontal resolution	200 km
Observation frequency	3 days
Random uncertainty	2 %
Systematic uncertainty	3 %
Stability	1-2 % / decade



## 5.2 Total ozone data product specifications

Product identifier	Horizontal resolution/Grid	Temporal resolution	File format
TC_L2_GOME	320x40 km <sup>2</sup>	3 days at equator	NetCDF
TC_L2_SCIA	60x30 km <sup>2</sup>	6 days at equator	NetCDF
TC_L2_GOME2	80x40 km <sup>2</sup>	Almost daily at equator	NetCDF
TC_L2_OMI	13x24 km <sup>2</sup> (at true nadir)	Daily at equator	NetCDF
TC_L2_OMPS	50x50 km <sup>2</sup>	Daily at equator	NetCDF
TC_L3_MRG	1°x1° (lat-long)	Monthly	NetCDF

## 5.3 File format specifications for total ozone data sets

### 5.3.1 Level 2 data format specification

#### *Description of Common and Product Specific Attributes*

Dimension and description of all variables contained in the L2 total ozone NetCDF files.  $N_p$  represents the total number of measurements for scanning instruments (GOME, SCIAMACHY, GOME-2) and the number of viewing lines for imager instruments (OMI).  $N_r$  is the number of rows for imager instruments (60 for OMI), and is 1 for scanner instruments.

Variable Name	Unit	Dimension	Description
<b>time</b>	Days	$N_p \times N_r$	Time of measurement in days since 1995-1-1 00:00:00
<b>time_of_measurement_string</b>	-	$N_p \times N_r \times 19$	String indicating the time of measurement at a glance: YYYYMMDDThhmmss.sss
<b>pixel_number</b>	-	$N_p \times N_r$	Ground pixel number
<b>state_number</b>	-	$N_p \times N_r$	State/MDR/Viewing line number. Only relevant for SCIAMACHY, GOME-2 and OMI.
<b>row_number</b>	-	$N_p \times N_r$	Row index number. Only relevant for OMI.
<b>pixel_type</b>	-	$N_p \times N_r$	Pixel type: 0 for forward pixels, 3 for backscan pixels
<b>latitude</b>	degree	$N_p \times N_r$	Latitude of the pixel center
<b>latitude_corner</b>	degree	$N_p \times N_r \times 4$	Latitudes of the pixel corners
<b>longitude</b>	degree	$N_p \times N_r$	Longitude of the pixel center



<b>longitude_corner</b>	degree	$N_p \times N_r \times 4$	Longitudes of the pixel corners
<b>solar_zenith_angle</b>	degree	$N_p \times N_r$	Solar zenith angle at the pixel center
<b>viewing_zenith_angle</b>	degree	$N_p \times N_r$	Viewing zenith angle at the pixel center.
<b>relative_azimuth_angle</b>	degree	$N_p \times N_r$	Relative zenith angle at the pixel center
<b>retrieval_mode_flags</b>	-	$N_p \times N_r$	retrieval mode: 0 for normal mode, 1 for snow/ice mode from cloud algorithm
<b>processing_flags</b>	-	$N_p \times N_r$	0: Nominal mode; 1: irregular L1 data - No retrieval; 2: Solar zenith angle larger than 89° - No retrieval; 3: No cloud data - No retrieval; 8: Forward model failure - No retrieval; 9: inversion failure - No retrieval; 21: Pixel affected by row anomaly - No retrieval; 22-24: Pixel might be affected by row anomaly - uncertain output
<b>atmosphere_mole_content_of_ozone</b>	DU	$N_p \times N_r$	Retrieved total ozone column
<b>atmosphere_mole_content_of_ozone_random_error</b>	DU	$N_p \times N_r$	Random error associated to the retrieved total column
<b>ozone_ghost_column</b>	DU	$N_p \times N_r$	Partial ozone column comprised between the ground and the effective surface
<b>fitted_ring_coefficient</b>	-	$N_p \times N_r$	Retrieved Ring scaling parameter
<b>effective_temperature</b>	°K	$N_p \times N_r$	Retrieved effective temperature
<b>cloud_area_fraction</b>	-	$N_p \times N_r$	Effective cloud fraction
<b>air_pressure_at_cloud_top</b>	Pa	$N_p \times N_r$	Cloud Top pressure
<b>cloud_albedo</b>	-	$N_p \times N_r$	Effective cloud top albedo provided by
<b>effective_scene_air_pressure</b>	Pa	$N_p \times N_r$	Pressure at the effective scene used for the retrieval
<b>effective_scene_albedo</b>	-	$N_p \times N_r$	Retrieved effective albedo of the scene
<b>surface_albedo</b>	-	$N_p \times N_r$	Minimum surface albedo at 335 nm from OMI LER climatology
<b>surface_altitude</b>	m	$N_p \times N_r$	Surface altitude extracted from GTOPO30



<b>rms</b>	-	$N_p \times N_r$	Root mean square of fit residuals
<b>reduced_chi_squared</b>	-	$N_p \times N_r$	Reduced chi-square of the fit
<b>nb_of_iterations</b>	-	$N_p \times N_r$	Number of iterations before convergence
<b>convergence_flag</b>	-	$N_p \times N_r$	Convergence flag: 0 for failure, 1 for success
<b>atmosphere_ pressure_grid</b>	Pa	$N_p \times N_r \times 15$	Pressure at levels defining the layers used in the forward model
<b>averaging_kernels</b>	-	$N_p \times N_r \times 14$	Averaging kernels in the layers of the forward model
<b>apriori_ozone_profile</b>	DU	$N_p \times N_r \times 14$	A-priori partial ozone columns in the layers of the forward model

### 5.3.2 Level 3 data format specification

#### *Description of Common Attributes*

Attribute	Description	Size	Value / Format
<b>Conventions</b>	NetCDF-CF convention version	8	'CF-1.4'
<b>Filename</b>	Name of the product file	TBD	Convention TBD
<b>Format</b>	NetCDF format version of the product file	4	Format M.NN where M=major, N=minor
<b>History</b>	Processing history of the product file	256	Free form
<b>processing_centre</b>	Centre where the product was generated	32	Free form
<b>archiving_centre</b>	Centre where the product is archived	32	Free form
<b>Instruments</b>	Comma separated list of instruments used for creating the product	64	e.g. 'GOME, SCIAMACHY, GOME-2'
<b>Satellites</b>	Comma separated list of satellite used for creating the product	64	e.g. 'ERS-2, ENVISAT, METOP-A'
<b>Level</b>	Processing level of the product	2	'L3'
<b>Projection</b>	Projection type of the product	32	'rectangular grid'
<b>Parameter</b>	Parameter of the Ozone-cci product	9	'O3TC', 'O3NP', 'O3LP' for ozone total column, ozone nadir profiles and ozone limb profiles respectively
<b>Revision</b>	Product revision (part of logical product identifier).	32	Free form
<b>processing_time</b>	Date and time (UTC) of product generation	14	Format YYYYMMDDHHMMSS
<b>base_product</b>	Name and version of the processor/algorithm used to generate the L2 parent product upon	32	Free form



	which the L3 product is based.		
<b>Processor</b>	Processor name and version used for generating the product	32	Free form
<b>Algorithm</b>	Algorithm name and version used for generating the product	32	Free form
<b>References</b>	Referencing information describing the product: document, web site, etc.	256	Free form
<b>Source</b>	Source of the product	32	'satellite observations'
<b>spatial_resolution</b>	Spatial resolution (in degrees square) of the product grid	4	e.g. '1.0', '0.5'
<b>temporal_resolution</b>	Temporal resolution of the product	8	'daily', 'weekly', 'monthly'
<b>start_time</b>	Start date and time (UTC) of temporal coverage	14	Format YYYYMMDDHHMMSS
<b>stop_time</b>	Stop date and time (UTC) of temporal coverage	14	Format YYYYMMDDHHMMSS

### *Description of Product Specific Attributes*

<b>Variable</b>	<b>NetCDF-CF standard name</b>	
Latitude	<b>Name</b>	latitude
	<b>Description</b>	Latitude is positive northward; its units of degree_north (or equivalent) indicate this explicitly. In a latitude-longitude system defined with respect to a rotated North Pole, the standard name of grid_latitude should be used instead of latitude. Grid latitude is positive in the grid-northward direction, but its units should be plain degree.
	<b>Unit/Range</b>	degrees from -90 to +90
Longitude	<b>Name</b>	longitude
	<b>Description</b>	Longitude is positive eastward; its units of degree_east (or equivalent) indicate this explicitly. In a latitude-longitude system defined with respect to a rotated North Pole, the standard name of grid_longitude should be used instead of longitude. Grid longitude is positive in the grid-eastward direction, but its units should be plain degree.
	<b>Unit/Range</b>	degrees from -180 to +180
time (1d array, short: time)	<b>Name</b>	Time
	<b>Description</b>	time since the specified reference time (NetCDF default)
	<b>Unit</b>	Depending on data version (e.g. daily aggregated or monthly mean): days or months since start time.
O3TC	<b>Name</b>	atmosphere_mass_content_of_ozone
	<b>Description</b>	"Content" indicates a quantity per unit area. The "atmosphere content" of a quantity refers to the vertical integral from the surface to the top of the atmosphere. For the content between specified levels in the atmosphere, standard names including content_of_atmosphere_layer are used. The chemical formula for ozone is O3.



	<b>Unit</b>	Dobson Units
O3TC_error	<b>Name</b>	n/a
	<b>Description</b>	Error associated to the ozone total column
	<b>Unit</b>	%

Note that latitude/longitude of the Ozone-cci products are given at the grid point centre.



## 6 Nadir ozone profile data products

Most CCMs resolve explicitly Earth atmosphere from the surface up to about 80 km altitude, i.e. the troposphere, the stratosphere, and most parts of the mesosphere. Typically the vertical resolution in the troposphere is below 1 km (about 500 m in the middle troposphere), it is about 1-2 km near the tropopause, with decreasing resolution in the stratosphere (e.g. 3-5 km in the middle stratosphere). Currently one of the further developments is to particularly increase the vertical resolution in the upper troposphere and lower stratosphere (UTLS) region, e.g. to reach a vertical resolution of about 500 m around the tropopause. The reason behind this is that the UTLS region is of particular importance for the Earth climate system including surface climate.

When comparing the user requirements as stated in the URD with publicly available data sets of ozone profiles the following characteristics are missing:

- Long-term period of data (requirements on time period)
- Consistent data set (requirements on stability)
- High quality data in the troposphere, UT/LS and middle atmosphere for the whole time period (requirements on systematic and random uncertainties)
- Unbiased data from multiple instruments (requirements on time period combined with the requirements on stability)

In the Ozone\_cci project, we will fulfil these requirements by using a single algorithm for the different UV-VIS instruments and include IASI ozone profiles from the thermal infrared. The UV-VIS algorithm uses an Optimal Estimation scheme and forward simulations of the nadir UV scattered radiance in the spectral interval from 270 to 340 nm to retrieve ozone profiles based on the BUV principle (see the Ozone\_cci ATBD for detailed algorithm description). In addition ozone profiles retrieved from IASI will be included. The profiles will be generated using the FORLI algorithm, to be used as the reference in upcoming versions of the IASI L2 PPF through activities covered by the O3M-SAF. The meteorological products needed for FORLI will be, at least in a first phase, from the latest available version of the IASI L2 PPF.

The data from the newly developed level-2 retrieval algorithms will be subsequently combined in level-3 and level-4 products after removing biases in the level-2 data between instruments. Meteorological information from the ECMWF ERA-Interim reanalysis will be used. This will lead to the generation of a data set covering the full data series in the second phase of the CCI programme.

In the following, the target uncertainties and the product specifications tables for Level 2, Level 3 and Level 4 products of the merged nadir ozone profiles are presented. Level-2, Level-3 and Level-4 data sets follow the user requirements for NetCDF CF standard.



## 6.1 Target uncertainties for CCI nadir ozone profile products

Quantity	Height range		
	Troposphere	UT/LS	Middle Atmosphere
Horizontal resolution	200 km	200 km	200 km
Vertical resolution	Tropospheric column	5 km	10 km
Observation frequency	3 days	3 days	3 days
Random uncertainty	20 %	15 %	15 %
Systematic uncertainty	20 %	15 %	15 %
Stability (after bias correction)	3 % / decade	3 % / decade	3 % / decade

Note: 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 coverage is global.

## 6.2 Nadir ozone profile data product specifications

Product identifier	Horizontal resolution	Vertical grid resolution	Vertical range	Temporal resolution	File format
NP_L2_GOME	960x80 km <sup>2</sup>	3-5 km	1000-0.01 hPa	3 days at equator	NetCDF
NP_L2_SCIA	State dependent	3-5 km	1000-0.01 hPa	6 days at equator	NetCDF
NP_L2_OMI	Viewing angle dep.	3-5 km	1000-0.01 hPa	1-2 days at equator	NetCDF
NP_L2_GOME2	160 x 160 km <sup>2</sup>	3-5 km	1000-0.01 hPa	1-2 days at equator	NetCDF
NP_L2_IASI	Viewing angle dep.: Varying from $36 \times \pi$ km <sup>2</sup> at nadir to $10 \times 20 \times \pi$ km <sup>2</sup> at the larger viewing angle	1 km	1000-2.5 hPa	Twice daily	NetCDF
NP_L3_MRG	1 x 1 °	3-5 km	1000-0.01 hPa	Monthly	NetCDF
NP_L4_MRG	1 x 1.5 °	1-2 km	1000-0.1 hPa	6 hours	NetCDF





## 6.3 File format specifications for nadir ozone profile data sets

### 6.3.1 Level 2 data format specification

This section describes the level 2 format in detail. The format includes full error characterisation information, averaging kernels, solution covariance and noise covariance, as well as the basic retrieved values.

The format of the Level 2 ozone profile product files is NetCDF. The values in all groups are taken from the level 1 or other input data files, or calculated by the program. The file includes output from both the retrieval algorithm and geolocation information, in addition to ancillary information such as surface pressure obtained from ERA-Interim analysis.

Modifications may be implemented in future in accordance with user needs or to improve consistency with other CCI products.

The following two tables contain the detailed data format for the nadir UV-VIS ozone profiles and IASI ozone profiles respectively.

#### UV-VIS data format

NCDF Variables			
Dataset name	Data type	Unit	Description
o3_nd	Float array, rank 2	cm-3	Ozone molecular number density Dimension = (n_profiles, n_o3_nd)
o3_vmr	Float array, rank 2	-	Ozone volume mixing ratio, (mole fraction of ozone in air) Dimension = (n_profiles, n_o3_vmr)
o3_error	Float array, rank 2	Percent	Retrieved ozone error Dimension = (n_profiles, n_o3_error)
o3_ap	Float array, rank 2	-	Ozone a priori volume mixing ratio (mole_fraction_of_ozone_in_air) Dimension = (n_profiles, n_o3_ap)
o3_ap_error	Float array, rank 2	Percent	ozone_a_priori_error Dimension = (n_profiles, n_o3_ap_error)
o3_sub_col	Float array, rank 2	Dobson Units	Ozone partial column (mole_content_of_ozone_in_atmosphere_layer) Dimension = (n_profiles, n_o3_sub_col)
o3_sub_col_error	Double array, rank 2	Dobson Units	Ozone partial column error (mole_content_of_ozone_in_atmosphere_layer) Dimension = (n_profiles, n_o3_sub_col_error)
o3_ap_sub_col	Double array,	Dobson Units	Ozone a priori partial column



	rank 2		(mole_content_of_ozone_in_atmosphere_layer) Dimension = (n_profiles, n_o3_sub_col)
o3_ap_sub_col_error	Double array, rank 2	Dobson Units	Ozone a priori partial column error (mole_content_of_ozone_in_atmosphere_layer) Dimension = (n_profiles, n_o3_ap_sub_col)
o3_tc	Float array, rank 1	Dobson Units	Total column ozone (atmosphere_mole_content_of_ozone) Dimension = n_profiles
o3_tc_error	Float array, rank 1	Dobson Units	Total column ozone error (atmosphere_mole_content_of_ozone) Dimension = n_profiles
o3_ap_tc_error	Double array, rank 1	Dobson Units	Ozone a priori total column error (atmosphere_mole_content_of_ozone)Dimension = n_profiles
o3_b1_sub_col	Double array, rank 2	Dobson Units	Band 1 ozone partial column (mole_content_of_ozone_in_atmosphere_layer) Dimension = (n_profiles, n_o3_b1_sub_col)
o3_b1_sub_col_error	Double array, rank 2	Dobson Units	Band 1 ozone partial column error (mole_content_of_ozone_in_atmosphere_layer) Dimension = (n_profiles, n_o3_b1_sub_col_error)
o3_b1_tc	Double array, rank 1	Dobson Units	Band 1 total ozone column (atmosphere_mole_content_of_ozone) Dimension = n_profiles
o3_b1_tc_error	Double array, rank 1	Dobson Units	Band 1 total ozone column error (atmosphere_mole_content_of_ozone) Dimension = n_profiles
nit	Long Int array, rank 1	-	Number of Iterations Dimension = n_profiles
b1nit	Long int array, Rank1	-	Band 1 number of iterations Dimension = n_profiles
Cost	Float array, rank 1	-	Final cost function value
ncost	Float array, rank 1	-	Normalised final cost function value
b1cost	Float array, rank 1	-	Band 1 cost function value Dimension = n_profiles



aconv	Intarray, rank 1	-	Convergence flag
b1conv	Long int array, rank 1	-	Band 1 convergence flag Dimension = n_profiles
achi	Long int array, rank 2	-	Chi squared flag Dimension = n_profiles
spre	Float, rank 1	hPa	Surface Pressure Dimension = n_profiles
levs	Float, rank 1	hPa	Pressure levels of retrieved ozone profiles Dimension = n_levels
lat	Float, rank 1	Degrees north	Latitude of ground pixel centre Dimension = n_profiles
lon	Float, rank 1	Degrees east	Longitude of ground pixel centre Dimension = n_profiles
ll	Float, rank 2	Degrees north/ degrees east	Latitude and longitude of ground pixel corners. [lat1,lon1,lat2,lon2,lat3,lon3,lat4,lon4] Dimensions = (n_profiles x n_ll)
pixno	Long Int, rank 1	-	Orbit ground pixel number ([scan line number * 100]+cross track scan position index) Dimension = n_profiles
sza	Float, rank 1	Degrees	Solar zenith angle Dimension = n_profiles
lza	Float, rank 1	Degrees	Line-of-sight zenith angle Dimension = n_profiles
time	Float, rank 1	Hours	Hours since 00:00.00hrs on date Dimension = n_profiles
scp	Short, rank 1	-	Across trak scan index Dimension = n_profiles
cloudf	Double, Rank 1	-	FRESCO effective cloud fraction
cloudp	Double, Rank 1	hPa	FRESCO cloud top pressure
clouda	Double, Rank 1	-	FRESCO cloud albedo
cloud_ffail	Short, Rank 1	-	FRESCO cloud fit fail indication
cloud_mode	Short,	-	FRESCO cloud fit mode



	Rank 1		
cloud_s6	Double, rank 1	-	Expected scaling of 0-6km sub column due to cloud Dimension = n_profiles
cloud_s12	Double, rank 1	-	Expected scaling of 0-12km sub column due to cloud Dimension = n_profiles
salb	Float, rank 1	-	Retrieved surface albedo Dimension = n_profiles
ring	Float, rank 1	-	Retrieved ring spectrum scaling parameter Dimension = n_profiles
xsect	Float, rank 1	-	Retrieved wavelength shift of absorptions cross sections Dimension = n_profiles
bro	Float, rank 1	-	BrO column average volume mixing ratio Dimension = n_profiles
bro_err	Float, rank 1	-	BrO column average volume mixing ratio error Dimension = n_profiles
no2	Float, rank 1	-	NO <sub>2</sub> column average volume mixing ratio Dimension = n_profiles
no2_err	Float, rank 1	-	NO <sub>2</sub> column average volume mixing ratio error Dimension = n_profiles
ch2o	Float, rank 1	-	CH <sub>2</sub> O column average volume mixing ratio Dimension = n_profiles
ch2o_err	Float, rank 1	-	CH <sub>2</sub> O column average volume mixing ratio error Dimension = n_profiles
rsf	Float, rank 1	-	Residual spectral pattern scaling factor Dimension = (n_profiles x n_misr)
slit	Float, rank 1	-	Slit function FWHM scaling parameter Dimension = n_profiles
misr	Float, rank 1	nm	Wavelength shift between radiance and irradiance spectra Dimension = (n_profiles x n_misr)
tsurf	Float, rank 1	K	Effective surface temperature Dimensions = (n_profiles, n_tsurf)
sx	Float arr, rank 3	cm-6	Ozone molecular number density solution covariance matrix Dimension = (n_profiles x n_sx_1, n_sx_0)
sn	Float array, rank 3	cm-6	Ozone molecular number density measurement noise covariance matrix Dimension = (n_profiles x n_sn_1 x n_sn_0)



ak	Float array, rank 3	-	Ozone molecular number density averaging kernel matrix Dimension = (n_profiles x n_ak_1, n_ak_2)
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### IASI data format

The FORLI algorithm for IASI operates with multiplication factors, with the a priori as reference, and the profile is adjusted in layer partial columns. The original output profile is in partial columns but will be provided here in the units needed to follow the general convention. The values in all groups are taken from the level 1 or other input data files, or calculated by the program. Further details, including on ancillary data, can be found in the ATBD.

Name	Type	Unit	Description
o3_sub_col	Float array	DU	<i>Ozone partial column vertical profile</i>
o3_sub_col_error	Float array	DU	<i>Vertical profile of total retrieved error</i>
o3_ap_sub_col	Float array	DU	<i>Ozone a priori partial columns vertical profile</i>
o3_tc	Float array	DU	<i>total column ozone</i>
ak	Float array	NA	<i>Averaging kernels matrix (molec cm-2/molec cm-2)</i>
sza	Float array	Degrees	<i>solar zenith angle</i>
cloudf	Float array	%	<i>EUMETSAT Cloud coverage in the pixel</i>
time	Int array	hhmmss	<i>Hour in the day</i>
lat	Float array	Degrees	<i>latitude of the ground pixel</i>
lon	Float array	Degrees	<i>longitude of the ground pixel</i>
dofs	Float array	NA	<i>Degrees Of Freedom of the Signal</i>
ret_flag	Int array	NA	<i>Retrieval quality flag</i>

### 6.3.2 Level 3 data format specification

#### *Description of Global Attributes*

The global attributes in the Level 3 files are compliant with the list provided in section 2.2 of the document “Guidelines for Data Producers - Climate Change Initiative Phase 1” (Bennett and James, 2013), repeated here for convenience:

- title (succinct description of the dataset)
- institution (where the data was produced, use names from CCI common vocabulary)
- source (original data source(s), e.g. MERIS RR L1B version 4.02). Multiple source datasets separated by commas.
- history (processing history of dataset)
- references (references to algorithm, ATBD, technical note describing dataset)
- tracking\_id (a UUID (Universal Unique Identifier) value)



- conventions (the CF Version)
- product\_version (the product version of this data file)
- summary (a paragraph describing the dataset)
- keywords (a comma separated list of key words and phrases)
- id
- naming authority (the combination of the naming authority and the id should be a globally unique identifier for the dataset)
- keywords\_vocabulary (if you are following a guideline for the words/phrases in your “keywords” attribute, put the name of that guideline here)
- cdm\_data\_type (the THREDDS data type appropriate for this dataset)
- comment (miscellaneous information about the data)
- date\_created (the date on which the data was created)
- creator\_name
- creator\_url
- creator\_email
- project (the scientific project that produced the data: “Climate Change Initiative – European Space Agency”)
- geospatial\_lat\_min (decimal degrees north, range -90 to +90)
- geospatial\_lat\_max (decimal degrees north, range -90 to +90)
- geospatial\_lon\_min (decimal degrees east, range -180 to +180)
- geospatial\_lon\_max (decimal degrees east, range -180 to +180)
- geospatial\_vertical\_min (assumed to be in metres above ground unless geospatial\_vertical\_units attribute defined otherwise)
- geospatial\_vertical\_max (assumed to be in metres above ground unless geospatial\_vertical\_units attribute defined otherwise)
- time\_coverage\_start (format `yyyymmddThhmmssZ`)
- time\_coverage\_end (format `yyyymmddThhmmssZ`)
- time\_coverage\_duration (should be an ISO8601 duration string)
- time\_coverage\_resolution (should be an ISO8601 duration string)
- standard\_name\_vocabulary (the name of the controlled vocabulary from which variable standard names are taken)
- license (describe the restrictions to data access and distribution)
- spatial\_resolution (a string describing the approximate resolution of the product. For example, “1.1km at nadir”)
- geospatial\_lat\_units
- geospatial\_lon\_units
- geospatial\_lon\_resolution
- geospatial\_lat\_resolution

### ***Description of Product Specific Datasets***

The datasets in the L3 files (version 2) are compliant with the NetCDF CF Metadata Conventions version 1.6 ([www.cfconventions.org](http://www.cfconventions.org)). Attached to each dataset are three attributes



describing the dataset: standard\_name (CF conventions standard name), long\_name and units. In the table below, only the datasets and the standard names are listed.

NetCDF variables			
Dataset name	Data type	Units	Description
lon	float, array, rank 1	degree East	longitude, from -180 (west) to +180 (east) given at gridcell centers. NetCDF dimension.
lat	float, array, rank 1	degree North	latitude, from -90 (south) to +90 (north) given at gridcell centers. NetCDF dimension.
layers	integer, array, rank 1	-	layer number, starting at 1. NetCDF dimension.
air_pressure	float, array, rank 1	hPa	air pressure at layer boundaries, replace the first element from this array with the corresponding surface pressure element. NetCDF dimension.
time	integer, array, rank 1	seconds	seconds since reference time, usually the start of the month. NetCDF dimension.
surface_pressure	float, array, rank 3	hPa	pressure at the bottom of the atmosphere with dimensions (time, lat, lon).
O3_du	float array, rank 4	DU	weighted average of the partial ozone columns (DU/layer) with dimensions (time, layers, lat, lon).
O3e_du	float array, rank 4	DU	uncertainty in the weighted average of the partial ozone columns (DU/layer) with dimensions (time, layers, lat, lon).
O3_du_tot	float array, rank 3	DU	total column: vertically integrated O3_du dataset (DU) with dimensions (time, lat, lon).
O3e_du_tot	float array, rank 3	DU	total column uncertainty: quadratically added o3e_du (DU) with dimensions (time, lat, lon).
O3_vmr	float array, rank 4	-	weighted average of the volume mixing ratio (ppmv) with dimensions (time, air_pressure, lat, lon).
O3e_vmr	float array, rank 4	-	uncertainty in the weighted average of the volume mixing ratio (ppmv) with dimensions (time, air_pressure, lat, lon).



O3_ndens	float array, rank 4	#molec cm <sup>-3</sup>	weighted average of the number density (#molecules/cm <sup>3</sup> ) with dimensions (time, air_pressure, lat, lon).
O3e_ndens	float array, rank 4	#molec cm <sup>-3</sup>	uncertainty in the weighted average of the number density (#molecules/cm <sup>3</sup> ) with dimensions (time, air_pressure, lat, lon).

### 6.3.3 Level 4 (assimilated) data format specification

#### *Description of Global Attributes*

The global attributes for the L4 files (version 3) are the same as for the L3 files. See the list in the previous section. In addition to those attributes a few deprecated attributes are present, which should not be used and might be removed in a future version of the dataset.

#### *Description of Product Specific Datasets*

Not all datasets in the L4 files have a standard name complying with the CF-conventions. This is the case with the datasets describing the vertical extent of the model field. In order to get a 3D pressure grid, one should do:  $p(k) = \text{Hybride\_coef\_a} + \text{Hybride\_coef\_b} * \text{Psurf}$ . The “Hybrid\_coef\_XXX” and “levels” datasets do not have a standard name, and in the table below, their long names have been listed.

NetCDF variables			
Dataset name	Data type	Units	Description
lon	float, array, rank 1	degree East	longitude, from -180 (west) to +180 (east) given at gridcell centers. NetCDF dimension.
lat	float, array, rank 1	degree North	latitude, from -90 (south) to +90 (north) given at gridcell centers. NetCDF dimension.
layers	integer, array, rank 1	-	layer number, starting at 1. NetCDF dimension.
levels	float, array, rank 1	-	levels = layers boundaries, starting at 1. NetCDF dimension.
time	integer, array, rank 1	hours	hours since reference time, usually midnight. NetCDF dimension.
Psurf	float, array, rank 3	Pa	surface air pressure with dimensions (time, lat, lon)





Temperature	float, array, rank 4	K	air temperature at layer centers with dimensions (time, layers, lat, lon)
Gph	float, array, rank 4	m	geopotential height at layer centers with dimensions (time, layers, lat, lon)
O3_vmr	float, array, rank 4	-	volume mixing ratio in ppv with dimensions (time, layers, lat, lon)
O3s_vmr	float, array, rank 4	-	uncertainty in the volume mixing ratio in ppv with dimensions (time, layers, lat, lon)
O3_dens	float, array, rank 4	#molec m <sup>-2</sup>	column density of ozone in #molecules m <sup>-2</sup> with dimensions (time, layers, lat, lon)
O3s_dens	float, array, rank 4	#molec m <sup>-2</sup>	uncertainty in the column density of ozone in #molecules m <sup>-2</sup> with dimensions (time, layers, lat, lon)
Hybride_coef_a	float, array, rank 1	Pa	Hybride half levels : $p(k) = \text{hyb\_a}(k) + \text{hyb\_b}(k) * ps$ [Pa]. Surface first.
Hybride_coef_b	float, array, rank 1	-	Hybride half levels : $p(k) = \text{hyb\_a}(k) + \text{hyb\_b}(k) * ps$ [Pa]. Surface first.
Hybride_coef_da	float, array, rank 1	Pa	surface first
Hybride_coef_db	float, array, rank 1	-	surface first
Hybride_coef_fa	float, array, rank 1	Pa	surface first
Hybride_coef_fb	float, array, rank 1	-	surface first
Cell_area	float, array, rank 1	m <sup>2</sup>	cell area per latitude with dimensions (lat)



## 7. Limb and occultation-type ozone profile data products

European limb-type data sets essentially rely on instrument being operated on the ENVISAT platform since 2002, i.e. MIPAS, GOMOS and SCIAMACHY, complemented by the ESA TPM missions OSIRIS, SMR and ACE-FTS. The questions associated with the short-term ozone changes (i.e. over the last decade) are primarily scientific in nature and are associated with improving our understanding of atmospheric processes by testing current models in relation to the various modes of internal variability (QBO, ENSO, etc.), or to external forcings such as volcanic eruptions, or the 27-day or 11-year cycles in solar variability. For all of these questions, accurate knowledge of the altitude, latitude, and seasonal dependence of the ozone response is required which all require measurements of high quality and a good error and information content characterisation.

In the Ozone\_cci project, we will fulfil these requirements through systematic improvement of the error characterisation for all ENVISAT instruments and some key ESA TPM sensors. As a result of the round robin exercise on 4 MIPAS processing algorithms performed in Phase 1, MIPAS data processed by KIT are selected. At the moment, a systematic use of the ERA-Interim meteorological dataset to specify temperature information in the retrievals is not applied. SCIAMACHY, GOMOS, OSIRIS and SMR are concerned by this issue, while MIPAS and ACE-FTS retrieve temperature profiles from observations. For SCIAMACHY, GOMOS and OSIRIS, the sensitivity to temperature mostly comes from the temperature dependence of the ozone absorption cross-sections in the region of the Huggins bands. Accordingly ozone retrievals are mainly sensitive to temperature in the upper stratosphere (30-60 km altitude range) and at these altitudes the corresponding uncertainty is estimated to be small, of the order of 0.5%. Such a sensitivity analysis will however be further refined and documented in the Ozone\_cci assessment phase, and the potential impact of making full use of consistent ERA-Interim meteorological data sets in the second phase of the CCI will be quantified.

As the first step to data harmonization, we have created the HARMOnized dataset of OZone profiles, HARMOZ (Sofieva et al., 2014). The harmonized dataset consists of original retrieved ozone profiles (Level 2) from each instrument, which are screened for invalid data by the instrument teams. While the original ozone profiles are presented in different units and on different vertical grids, the harmonized dataset is given on a common pressure grid in netCDF-4 format. The pressure grid corresponds to vertical sampling of ~1 km below 20 km and 2–3 km above 20 km. The vertical range of the ozone profiles is specific for each instrument, thus all information contained in the original data is preserved. Provided altitude and temperature profiles allow the representation of ozone profiles in number density or mixing ratio on a pressure or altitude vertical grid. Geolocation, uncertainty estimates and vertical resolution are provided for each profile. For each instrument, optional parameters, which are related to the data quality, are also included. The details on the dataset can be found in (Sofieva et al., 2014). The parameters included in the dataset are presented in (Sofieva et al., 2014) and can be found in the Section 7.2



In Phase 1, the following Level 3 ozone profiles datasets based on limb and occultation data have been produced:

- Monthly zonal mean data from individual instruments (all years)
- Merged monthly zonal mean ozone profiles (years 2007-2008)
- Semi-monthly mean ozone profiles with resolved longitudinal structure (years 2007-2008)

The details of the datasets and the data format are described below and at the Ozone\_cci web-page. They follow the user requirements for NetCDF format and CF metadata convention.

## 7.1 Target uncertainties for CCI limb-type ozone profile products

Limb and occultation-type ozone profile ECV data products result from the merging of 4 instruments datasets: MIPAS, SCIAMACHY, GOMOS, and OSIRIS (possibly complemented by data from the SMR and ACE-FTS instruments). Within the merging process, non-compliant characteristic of any participating dataset is translated into error terms, leading to a corresponding smaller weight to non-reliable measurements. As a result the merged data product is designed to retain the best performance of all contributing sensors. The target error estimate given below is based on this principle.

Quantity	Height range		
	Lower stratosphere	Middle Atmosphere	Mesosphere
Horizontal resolution	250-500 km	500-1000 km	<i>TBD (from URD)</i>
Vertical resolution	2-4 km	3-4 km	<i>TBD (from URD)</i>
Observation frequency	3 days	3 days	<i>TBD (from URD)</i>
Uncertainty in height registration	50-200 m	50-200 m	<i>TBD (from URD)</i>
Random uncertainty	8-10 %	8-10 %	<i>TBD (from URD)</i>
Systematic uncertainty	15 %	15 %	<i>TBD (from URD)</i>
Stability	1-2 % / decade	1-2 % / decade	<i>TBD (from URD)</i>

Note: the lower stratosphere extends from about 15 to 25 km, and the middle atmosphere extends from about 25 to 60 km altitude. The coverage is global.

## 7.2 HARMOZ data product specifications

HARMOZ ozone profiles are structured in folders corresponding to each instrument. Each folder contains monthly data files with self-explanatory names: ESACCI-OZONE-L2-LP-III\_SSSS-PP\_VV-YYYYMM-Z.nc, where L2=Level 2, LP=Limb Product, III= instrument, SSSS=satellite, PP=processing center, VV= processor version, YYYY= year, MM=month,



Z=file version. For example, the file ESACCI-OZONE-L2-LP-GOMOS\_ENVISAT-IPF\_V6-200801-fv0004.nc contains GOMOS ozone profiles for January 2008.

Each file contains the mandatory parameters, which are the same for all instruments (Table 1). The files contain also optional instrument-specific parameters (Table 2), which might be related to the data quality.

**Table 1 Mandatory parameters in the HARMOZ netcdf files.  $N_{alt}$  and  $N_{prof}$  denote the number of pressure levels and the number of profiles, respectively**

<i>Parameter and unit</i>	<i>Dimensions</i>	<i>Description</i>
time(days since 1900-01-01 00:00:00)	$N_{prof} \times 1$	The parameter to index the profiles
air_pressure (hPa)	$N_{alt} \times 1$	The vertical coordinate
altitude (km)	$N_{alt} \times N_{prof}$	The geometric altitude above the mean sea-level
latitude (degree_north)	$N_{prof} \times 1$	Latitude of each profile
longitude (degree_east)	$N_{prof} \times 1$	Longitude of each profile
mole_concentration_of_ozone_in_air (mol/cm <sup>3</sup> )	$N_{alt} \times N_{prof}$	Vertical profiles of ozone. Number density (cm <sup>-3</sup> ) is acquired by multiplying the variable with Avogadro constant $N_A=6.02214e23 \text{ mol}^{-1}$
mole_concentration_of_ozone_in_air_standard_error (mol/cm <sup>3</sup> )	$N_{alt} \times N_{prof}$	Uncertainty (random error) associated with the ozone profiles
vertical_resolution (km)	$N_{alt} \times N_{prof}$ or $N_{alt} \times 1$	FWHM of the averaging kernel
air_temperature (K)	$N_{alt} \times N_{prof}$	Temperature profiles at the locations of measurements, for conversion from concentration to mixing ratio



**Table 2. Optional parameters in HARMOZ netcdf files  $N_{alt}$  and  $N_{prof}$  denote the number of pressure levels and the number of profiles, respectively**

	<i>Parameter and unit</i>	<i>Dimensions</i>	<i>Description/comment</i>
GOMOS	orbit_number	$N_{prof} \times 1$	Envisat orbit number
	star_number	$N_{prof} \times 1$	Star number in GOMOS catalogue
	star_magnitude	$N_{prof} \times 1$	Star visual magnitude
	star_temperature (K)	$N_{prof} \times 1$	Star effective temperature
	obliquity (deg)	$N_{prof} \times 1$	Obliquity of occultation: the angle between the orbital plane and the line of sight
	sza (deg)	$N_{prof} \times 1$	solar zenith angle at tangent point
	Chi2	$N_{alt} \times N_{prof}$	Profiles of normalized $\chi^2$ - statistics. Usually close to 1. Large values indicate problems with retrievals
	illumination_condition_flag	$N_{prof} \times 1$	0-full dark, 3-straylight, 2- twilight, 4- straylight&twilight.
	SAA_flag	$N_{prof} \times 1$	The indicator showing that the data might be affected by the Southern Atlantic Anomaly (cosmic rays); 0- no, 1- yes
SCIAMACHY	orbit_number	$N_{prof} \times 1$	Envisat orbit number
	state_id	$N_{prof} \times 1$	State ID of the SCIA measurement
	height_sat (km)	$N_{prof} \times 1$	Satellite altitude above the sea-level, for each profile
	radius_earth (km)	$N_{prof} \times 1$	The Earth radius at locations above the tangent points
	sza_tanpnt (deg)	$N_{prof} \times 1$	solar zenith angle at tangent point
	pixel_lat (degree_north)	$N_{prof} \times 4$	the ground latitudes of the four corners of the limb scan pixel
	pixel_lon (degree)	$N_{prof} \times 4$	the ground longitude of the four corners of the limb scan pixel
	total_ozone_column (mm)	$N_{prof} \times 1$	Total ozone column for each profile; 1mm=100 DU (Dobson Unit)
systematic_error (%)	$N_{alt} \times N_{prof}$	Systematic errors derived from parameter deviation simulation (see ozone-CCI ATBD)	
MIPAS	apriori_temperature (K)	$N_{alt} \times N_{prof}$	temperature profiles at locations of measurements based on ECMWF and MSIS data
	geo_id	$N_{prof} \times 22$	MIPAS geolocation identifier formatted as XXXXX_YYYYMMDDThhmmssZ where XXXXX=orbit, YYYY=year, MM=month, DD=day, hh=hour, mm=minute, ss=second
	orbit_number	$N_{prof} \times 1$	Envisat orbit number
	sza(deg)	$N_{prof} \times 1$	Solar zenith angle
	chi2	$N_{prof} \times 1$	Normalized $\chi^2$ - value of retrievals
	dof	$N_{prof} \times 1$	degrees of freedom of target retrieval
	rms (nW/cm/sr)	$N_{prof} \times 1$	root mean square of residual spectra
OSIRIS	scan_number	$N_{prof} \times 1$	OSIRIS scan number
	albedo	$N_{prof} \times 1$	Retrieved albedo
	ssa (deg)	$N_{prof} \times 1$	Solar scattering angle
	sza(deg)	$N_{prof} \times 1$	Solar zenith angle
	optics_temperature (K)	$N_{prof} \times 1$	Average optics box temperature
SMR	quality	$N_{prof} \times 1$	Quality flag 0: best quality, 4: tolerable
	solar_zenith_angle (deg)	$N_{prof} \times 1$	
	local_solar_time (h)	$N_{prof} \times 1$	
	measurement_response	$N_{alt} \times N_{prof}$	Proportion of measurement; measurements with weak influence of a priori have measurement response close to 1.
	scaled_potential_vorticity ( $K m^2 kg^{-1} s^{-1}$ )	$N_{alt} \times N_{prof}$	Profiles of potential vorticity (Lait, 1994) scaled at 475 K potential temperature level



	equivalent_latitude (deg)	$N_{alt} \times N_{prof}$	Profiles of equivalent latitude at locations of measurements
ACE-FTS	beta_angle (deg)	$N_{prof} \times 1$	$\beta$ -angle is defined as the angle between the orbit plane of ACE-FTS and the vector from the Sun. It is a proxy for vertical resolution.

### 7.3 Limb-type ozone profile Level 3 data product specifications

#### Monthly zonal mean data from individual instruments

The monthly zonal mean (MZM) data set provides ozone profiles averaged in 10° latitude zones from 90°S to 90°N, for each month. The monthly zonal mean data are structured into yearly netcdf files, for each instrument separately. The self-explaining name indicates the instrument and the year. For example, the file “ESACCI-OZONE-L3-LP-GOMOS\_ENVISAT-MZM-2008.nc” contains monthly zonal mean data for GOMOS in 2008. The variables that are included into netcdf files are collected in Table 3.

**Table 3 The variables in MZM netcdf files.  $N_{month}$ ,  $N_{alt}$ ,  $N_{lat}$  are number of months, pressures levels and latitude zones, respectively.**

<i>Parameter and unit</i>	<i>Dimension</i>	<i>Description</i>
	$S$	
Time	$N_{month} \times 1$	The parameter to index the months. The time is assigned to the middle of month and presented in “days since 1900-01-01 00:00:00”
air_pressure (hPa)	$N_{alt} \times 1$	The vertical coordinate
approximate_altitude (km)	$N_{alt} \times 1$	Approximate altitude at pressure levels computed as $z = 16 \log_{10}(1013/P)$ , $P$ is pressure in hPa
latitude_centers (degree_north)	$N_{lat} \times 1$	Centers of latitude bins: -85°: 10°:85°
ozone_mixing_ratio	$N_{lat} \times N_{alt} \times N_{m}$ onth	Monthly zonal mean ozone mixing ratio vertical profiles
ozone_mole_concentration (mol/cm <sup>3</sup> )	$N_{lat} \times N_{alt} \times N_{m}$ onth	Monthly zonal mean ozone mole concentration vertical profiles
standard_error_of_the_mean (%)	$N_{lat} \times N_{alt} \times N_{m}$ onth	Uncertainty of the monthly zonal mean*
sample_standard_deviation (%)	$N_{lat} \times N_{alt} \times N_{m}$ onth	Sample standard deviation in 1 month $\times 10^\circ$ spatio-temporal bins, for each pressure level*
mean_uncertainty_estimate (%)	$N_{lat} \times N_{alt} \times N_{m}$ onth	Monthly zonal mean of error estimates
inhomogeneity_in_time	$N_{lat} \times N_{alt} \times N_{m}$ onth	Inhomogeneity measure in time*
inhomogeneity_in_latitude	$N_{lat} \times N_{alt} \times N_{m}$ onth	Inhomogeneity measure in latitude*

\*The definitions of the parameters can be found in the “Data description and user manual” document available at <http://www.esa-ozone-cci.org/?q=node/166>



### Merged monthly zonal mean ozone profiles

The merged monthly zonal mean data (MMZM hereafter) include merged ozone profiles in 10° latitude zones for each month, at ozone-CCI pressure grid from 250 hPa to 1 hPa, and the parameters, which characterize the uncertainty of the merged profiles. In Phase I, the dataset has been created for 2 years, 2007 and 2008.

The merged monthly zonal mean data are structured into monthly netcdf files with self-explanatory names. For example, the file “ESACCI-OZONE-L3-LP-MERGED-MZM-200801-fv0002.nc” contains merged monthly zonal mean data for January 2008. In addition to the variables of the merged data, the profiles from individual instruments with their uncertainty parameters are also included (for the altitude range 250-1 hPa used in data merging). The variables included into netcdf files are collected in Table 4.

**Table 4. The variables in MMZM netcdf files**

	<i>Parameter and unit</i>	<i>Dimensions</i>	<i>Description</i>
General parameters	air pressure (hPa)	$N_{alt} \times 1$	The vertical coordinate
	approximate_altitude (km)	$N_{alt} \times 1$	Approximate altitude at pressure levels computed as $z = 16 \log_{10}(1013/P)$ , $P$ is pressure in hPa
	latitude_centers (degrees_north)	$N_{lat} \times 1$	Centers of latitude bins: -85°: 10°:85°
	instruments	$N_{instru} \times 1$	A dimension for individual datasets, instrument order 1-GOMOS, 2-MIPAS, 3-SCIAMACHY, 4-OSIRIS, 5-ACE-FTS, 6-SMR
Merged data	merged_ozone_vmr	$N_{lat} \times N_{alt}$	Merged monthly zonal mean ozone mixing ratio vertical profiles
	merged_ozone_concentration (mol/cm <sup>3</sup> )	$N_{lat} \times N_{alt}$	Vertical profiles of merged monthly zonal mean ozone mole concentration. Number density (cm <sup>-3</sup> ) is acquired by multiplying the variable with Avogadro constant $N_A = 6.02214e23 \text{ mol}^{-1}$
	uncertainty_of_merged_ozone (%)	$N_{lat} \times N_{alt}$	Uncertainty of the merged data *
Individual datasets	ozone_vmr	$N_{lat} \times N_{alt} \times N_{instru}$	Monthly zonal mean ozone mixing ratio vertical profiles for individual instruments
	ozone_mole_concentration (mol/cm <sup>3</sup> )	$N_{lat} \times N_{alt} \times N_{instru}$	Monthly zonal mean ozone mole concentration vertical profiles for individual instruments.
	standard_error_of_the_mean (%)	$N_{lat} \times N_{alt} \times N_{instru}$	Uncertainty of the monthly zonal mean for individual datasets*
	sampling_error (%)	$N_{lat} \times N_{alt} \times N_{instru}$	Sampling error for individual datasets*.
	total_error (%)	$N_{lat} \times N_{alt} \times N_{instru}$	Total uncertainty of monthly zonal mean data from individual instruments*

\*The definitions of the parameters can be found in the Data description and user manual” document available at <http://www.esa-ozone-cci.org/?q=node/167>.

### Semi-Monthly Mean dataset

The Merged Semi-Monthly Mean (MSMM) dataset is created using measurements from limb sensors participating in Ozone\_cci project, for years 2007-2008 (Phase 1).





First, the ozone profiles from individual instruments are averaged in  $10^\circ \times 20^\circ$  latitude-longitude zones over half-month time intervals, and then merged.

The merged semi-monthly mean ozone profiles are structured into yearly netcdf files with self-explanatory names. For example, the file “ESACCI-OZONE-L3-LP-SMM-2008-fv0002.nc” contains the semi-monthly mean ozone profiles for January 2008. In addition to the variables of the merged data, the profiles from individual instruments with their uncertainty parameters are also included (for the altitude range 250-1 hPa used in data merging). The variables included into netcdf files are collected in Table 5.

**Table 5. The variables in MSMM netcdf files.  $N_{alt}$  is number of pressure levels,  $N_{lat}$  and  $N_{lon}$  are numbers of latitude and longitude bins, respectively,  $N_{time}$  is number of temporal intervals and  $N_{instru} = 6$  is number of instruments.**

	<i>Parameter and unit</i>	<i>Dimensions</i>	<i>Description</i>
General parameters	air pressure (hPa)	$N_{alt} \times 1$	The vertical coordinate
	approximate_altitude (km)	$N_{alt} \times 1$	Approximate altitude at pressure levels computed as $z = 16 \log_{10}(1013 / P)$ , $P$ is pressure in hPa
	latitude_centers (degree_north)	$N_{lat} \times 1$	Centers of latitude bins: $-85^\circ: 10^\circ: 85^\circ$
	longitude_centers (degree_east)	$N_{lon} \times 1$	Centers of longitude bins: $-170^\circ: 20^\circ: 170^\circ$
	time	$N_{time} \times 1$ ( $24 \times 1$ )	Central date for each half of month, expressed as days since 1 January 1900
	instruments	$N_{instru} \times 1$	A dimension for individual datasets, instrument order 1-GOMOS, 2-MIPAS, 3-SCIAMACHY, 4-OSIRIS, 5-ACE-FTS, 6-SMR
Merged data	merged_ozone_vmr	$N_{lat} \times N_{lon} \times N_{alt} \times N_{time}$	Merged semi-monthly zonal mean ozone mixing ratio vertical profiles
	merged_ozone_concentration (mol/cm <sup>3</sup> )	$N_{lat} \times N_{lon} \times N_{alt} \times N_{time}$	Vertical profiles of merged semi-monthly zonal mean ozone mole concentration. Number density (cm <sup>-3</sup> ) is acquired by multiplying the variable with Avogadro constant $N_A = 6.02214 \times 10^{23} \text{ mol}^{-1}$
	uncertainty_of_merged_ozone (%)	$N_{lat} \times N_{lon} \times N_{alt} \times N_{time}$	Uncertainty of the merged data*
Individual datasets	ozone_vmr	$N_{lat} \times N_{lon} \times N_{alt} \times N_{time}$	Semi-monthly zonal mean ozone mixing ratio vertical profiles for individual instruments
	ozone_mole_concentration (mol/cm <sup>3</sup> )	$N_{instru} \times N_{lat} \times N_{lon} \times N_{alt} \times N_{time}$	Semi-monthly zonal mean ozone mole concentration vertical profiles for individual instruments.
	standard_error_of_the_mean (%)	$N_{instru} \times N_{lat} \times N_{lon} \times N_{alt} \times N_{time}$	Uncertainty of the semi-monthly zonal mean for individual datasets*
	sampling_error (%)	$N_{instru} \times N_{lat} \times N_{lon} \times N_{alt} \times N_{time}$	Sampling error for individual datasets*.
	total_error (%)	$N_{time} \times N_{lat} \times N_{lon} \times N_{alt} \times N_{instru}$	Total uncertainty of semi-monthly zonal mean data from individual instruments*
	inhomogeneity_in_longitude	$N_{instru} \times N_{lat} \times N_{lon} \times N_{alt} \times N_{time}$	Inhomogeneity measure in longitude*
	inhomogeneity_in_latitude	$N_{instru} \times N_{lat} \times N_{lon} \times N_{alt} \times N_{time}$	Inhomogeneity measure in latitude*
	inhomogeneity_in_time	$N_{instru} \times N_{lat} \times N_{lon} \times N_{alt} \times N_{time}$	Inhomogeneity measure in time*





\*The definitions of the parameters can be found in the Data description and user manual” document available at <http://www.esa-ozone-cci.org/?q=node/168>

## **7.4 UTLS data product specifications**

*To be specified in year 2*

## **7.5 Mesosphere data product specifications**

*To be specified in year 2*



## 8. Tropospheric data products

### 8.1 Target uncertainties for CCI tropospheric ozone data products

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

### 8.2 Tropospheric ozone data product specifications

Product identifier	Horizontal resolution/Grid	Temporal resolution	File format
TROPOL_I4_MRG_KNMI	3° × 2° (lon × lat)	month	NetCDF
			NetCDF
			NetCDF
			NetCDF
			NetCDF
			NetCDF



### 8.3 File format specifications for tropospheric ozone data sets

TROPOL_L4_MRG_KNMI NetCDF variables			
Dataset name	Data type	Units	Description
lon	float, array, rank 1	degree East	longitude, from -180 (west) to +180 (east) given at gridcell centers. NetCDF dimension.
lat	float, array, rank 1	degree North	latitude, from -90 (south) to +90 (north) given at gridcell centers. NetCDF dimension.
levels	float, array, rank 1	-	levels = layers boundaries, starting at 1. NetCDF dimension.
time	integer, array, rank 1	seconds	seconds since reference time, usually the start of the month. NetCDF dimension.
psurf	float, array, rank 3	hPa	air pressure at the bottom of the atmosphere with dimensions (time, lat, lon).
trop_def	string	-	tropopause definition used to generate the 'trop_' products.
trop_hpa	float, array, rank 3	hPa	air pressure at the top of the troposphere with dimensions (time, lat, lon).
trop_du	float array, rank 3	DU	weighted average of the partial tropospheric ozone column with dimensions (time, lat, lon).
trop_du_e	float array, rank 3	DU	uncertainty in the weighted average of the partial tropospheric ozone column with dimensions (time, lat, lon).



## 8 References

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## 9 Acronyms

ATBD	Algorithm Theoretical Basis Document
BIRA-IASB	Belgian Institute for Space Aeronomy
CCI	Climate Change Initiative
CCM	Chemistry-Climate Model
CTM	Chemistry-Transport Model
CMUG	Climate Modeling User Group
CRG	Climate Research Group
DARD	Data Access Requirements Document
DLR	German Aerospace Centre
DU	Dobson Unit
ECMWF	European Centre for Medium-range Weather Forecast
ECV	Essential Climate Variable
ENVISAT	Environmental Satellite (ESA)
ESA	European Space Agency
EUMETSAT	European Organisation for the Exploitation of Meteorological Satellites
FMI	Finnish Meteorological Institute
GCOS	Global Climate Observation System
GDP	GOME Data Processor
GOME	Global Ozone Monitoring Experiment (aboard ERS-2)
GOME-2	Global Ozone Monitoring Experiment – 2 (aboard MetOp-A)
GOMOS	Global Ozone Monitoring by Occultation of Stars
IUP-Bremen	Institute of Environmental Physics, University of Bremen
KIT	Karlsruhe Institute of Technology
KNMI	Royal Netherlands Meteorological Institute
LATMOS	Laboratoire Atmosphères, Milieux, Observations Spatiales
MetOp	Meteorological Operational Platform (EUMETSAT)
MIPAS	Michelson Interferometer for Passive Atmospheric Sounding
OMI	Ozone Monitoring Instrument (aboard EOS-Aura)
OSIRIS	Optical and Spectroscopic Remote Imaging System (aboard Odin)
PSD	Product Specification Document
RAL	Rutherford Appleton Laboratory
SASK	Saskatchewan University
SCIAMACHY	Scanning Imaging Absorption Spectrometer for Atmospheric Cartography
TBD	To be determined
URD	User Requirement Document
WMO	World Meteorological Organization