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Ozone-cci



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1 Introduction

1.1 Purpose and scope

This Product Validation Plan (PVP) summarises the validation requirements for three ozone Essential Climate Variable (ECV) data products of the ESA-funded Ozone_cci project, namely, total ozone columns, nadir-based ozone profiles, and limb-based ozone profiles. This plan is expected to evolve and shall be updated as the definition of the ozone ECV product consolidates and the understanding of algorithmic issues improves.

1.2 Document overview

The Ozone cci Product Validation Plan is organised as follows:

- o Chapter 1 contains this introduction describing the scope of the document.
- o Chapter 2 lists applicable and reference documents.
- o Chapter 3 reproduces the user requirements against which ECV products should be validated.
- Chapter 4 defines the Evaluation Protocol for the final ECV data product. It starts with generic principles of the ECV validation and explains the specifics with regard to validation of the three different ozone ECVs.
- O Chapter 5 defines the Round Robin Evaluation Protocol and the Interim Evaluation Protocol. The Round Robin Evaluation Protocol describes evaluation procedures and criteria supporting the selection of a retrieval algorithm when several algorithms are in competition for the same ECV data product. The Interim Evaluation Protocol defines the minimum set of validation tasks to be carried out when an algorithm has been selected, before it is applied to the entire level-1 data record. The Interim Evaluation Protocol has also to be applied when an algorithm selected for a given level-1 data set is transferred to the analysis of another level-1 data set, either from the same satellite instrument or from another one.
- o Chapter 6 addresses validation and quality control standards: sustainable archiving and traceability of the validation process and of validation results, quality control metadata and criteria, and compliance with international standards and with the EC Directive INSPIRE.
- o Chapter 7 checks the compliance of this document with requirements expressed in the Statement Of Work of the CCI programmes and its ozone related annexes.
- o Chapter 8 defines the recommended terminology, abbreviations and acronyms.



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2 Applicable and reference documents

2.1 Applicable documents

- [RD1] <u>CCI SoW</u>: ESA Climate Change Initiative Phase 1 Scientific User Consultation and Detailed Specification Statement of Work, EOP-SEP/SOW/0031-09/SP, Issue 1.4 / Revision 1, 52 pp., 09/11/2009 + Annex B: Ozone ECV (Ozone_cci).
- [RD2] <u>CCI Baseline Proposal</u>: ESA Climate Change Initiative Phase 1 Scientific User Consultation and Detailed Specification Essential Climate Variable: Ozone Baseline Proposal Volume I: Technical and Management Proposal, Ref. 58.805/21.0/54.49, 252 pp., 04/03/2010.

2.2 Reference documents

2.2.1 Requirement documents

- [RD3] <u>CMUG</u>: Requirement Baseline Document, Deliverable 1.2, Climate Modelling User Group, version 1.3, November 2010.
- [RD4] <u>DARD</u>: Ozone CCI Data Access Requirement Document, Version 1, Issue 1.0, Ozone cci DARD 1.1, April 29, 2011.
- [RD5] <u>IGACO</u>: 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), 2004.
- [RD6] <u>URD</u>: Ozone CCI User Requirement Document, Version 1, Issue 1.0, 26 pp., Ozone_cci_URD_1.0, April 4, 2011.
- [RD7] <u>WMO rolling requirements</u>: 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

2.2.2 Standards and framework documents

- [RD8] CDRH: Center for Devices and Radiological Health (CDRH), General Principles of Software Validation; Final Guidance for Industry and FDA Staff, CBER CDRH/OC Doc. N. 938, January 11, 2002. Publicly available via http://www.fda.gov/MedicalDevices/DeviceRegulationandGuidance/
- [RD9] <u>CEOS</u>: Committee on Earth Observation Satellites (CEOS): Terms and Definitions and other documents and resources, publicly available on http://calvalportal.ceos.org
- [RD10] <u>GUM</u>: Joint Committee for Guides in Metrology (JCGM/WG 1) 100:2008, Evaluation of measurement data Guide to the expression of uncertainty in a measurement (GUM), http://www.bipm.org/utils/common/documents/jcgm/JCGM_100_2008_E.pdf
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- [RD14] <u>VIM</u>: Joint Committee for Guides in Metrology (JCGM/WG 2) 200:2008 & ISO/IEC Guide 99-12:2007, International Vocabulary of Metrology Basic and General Concepts and Associated Terms (VIM), http://www.bipm.org/en/publications/guides/vim.html
- [RD15] WMO Quality Management Framework (QMF), home page at http://www.wmo.int/pages/prog/www/QMF-Web/home.html
- [RD16] QA4EO A Quality Assurance framework for Earth Observation, established by the CEOS. It consists of ten distinct key guidelines linked through an overarching document (the QA4EO Guidelines Framework) and more community-specific QA4EO procedures, all available on http://qa4eo.org/documentation.html A short QA4EO "user" guide has been produced to provide background into QA4EO and how one would start implementing it (http://qa4eo.org/docs/QA4EO guide.pdf)
- [RD17] ISO Quality Management Principles available at http://www.iso.org/iso/iso9000-14000/understand/qmp.html
- [RD18] NetCDF Climate and Forecast Metadata Convention, http://cf-psmdi.llnl.gov
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- [RD36] De Clercq, C., J.-C. Lambert, J. Granville, P. Gerard, A. Kaifel, J. Kaptur, B. Mijling, O. tuinder, R. van Oss, and C. Zehner, CHEOPS-GOME, Geophysical information content and validation of ERS-2 GOME ozone profile data records, IASB/ESA Technical Note TN-IASB-GOME1-CHEOPS-01, Issue 1, Revision B, 122 pp., 20 December 2007.



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3 User requirements

3.1 General requirements

ECVs produced within the Ozone_CCI project consist in (i) a column integrated ozone data product, (ii) ozone profile data derived from nadir measurements, and (iii) ozone profile data derived from limb measurements. For each of these products the Ozone_CCI User Requirement Document (URD) [RD6] defines climate user requirements, based on the ozone requirements of the Global Climate Observing System, the CCI Climate Modelling User Group (CMUG) [RD3], the Integrated Global Atmospheric Chemistry Observation theme (IGACO) of the Integrated Global Observing Strategy (IGOS) [RD5], and the WMO rolling requirements [RD7]. The Ozone-CCI Validation Team (VALT) has translated these URD requirements into validation requirements.

The first category of user requirements addresses classical error bars. In the case of total ozone column TOC (expressed in DU) the error will be given as a delta total ozone value in DU (δ TOC), usually equal to 2% or 3%, such that TOC \pm δ TOC represents a \pm 68% confidence interval. This δ TOC value contains a systematic term and a random term, corresponding to classical bias and precision (1 σ standard deviation or equivalent) estimates. Validation is expected to verify the bias and precision estimates provided by the ECV retrieval teams. This verification must ensure that these quality indicators, which usually vary with several parameters of the measurement and the retrieval, remain within the acceptable ranges defined in URD. In the case of ozone profiles two error bars are required, one representing an altitude range (\pm 500m for limb retrievals), the other representing a volume mixing ratio range (requirements between 8% and 20%), and both representing a \pm 68% confidence interval. Figure 1 illustrates these requirements. URD specifies that from a climate modelling perspective it would be acceptable to translate the height registration error into an additional mixing ratio error. Assessment of the error bar on altitude depends directly on the ECV and will be addressed in dedicated sections.

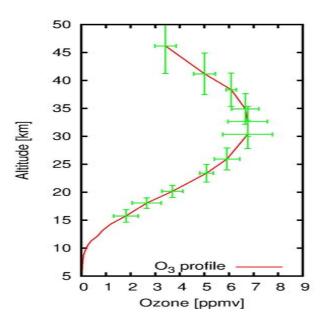


Figure 1 Illustration of an ozone profile and the reporting of errors (from URD 1.0, 2011)



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The second category of user requirements addresses (i) the temporal and spatial domains over which, and (ii) the associated temporal and spatial resolutions at which, data quality must meet the first category of user requirements:

- Temporal domain and sampling: continuous coverage with 3 days of observation frequency over the decadal range and beyond, with long-term stability of 1%-3%/decade to allow trend detection, and with maximum uncertainty on interannual variability, annual cycle and shorter term variability ranging from 2-3% for total ozone data up to 20% for tropospheric ozone data.
- o Geographical domain: global, regional, latitude-height monthly mean cross-sections.
- o Horizontal resolution requirements: from 20 km to 300 km depending on the ECV.
- Vertical range and sensitivity: requirements reflect the vertical structure of ozone changes, namely total ozone column (TOC), total tropospheric ozone column (TTOC), and ozone in the lower troposphere (LT), upper troposphere (UT), lower stratosphere (LS), upper stratosphere and mesosphere (USM).
- Vertical resolution: depending on the ECV.

Other user requirements fall into the following categories:

- Level of the ECV data set: off-line homogenized Level-2 time series for process evaluations on time scales spanning from hours/days to months/years, and homogenized multi-instrument longterm data sets for ozone-climate interactions (Level-3 and Level-4).
- o Continuity of user requirements between data levels, e.g., aggregated multi-sensor Level-3 products should retain 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.
- o Requirements for ancillary data: cloud information per pixel (including cloud fraction, cloud height, cloud albedo) and surface information per pixel (surface albedo).
- Data format and metadata requirements.
- Visualisation requirements.

Hereafter we reproduce the user requirements as described in version 1.0 of the URD (Tables 5.2.1 to 5.4.2), against which ECV products have to be verified and/or validated. For each ECV the tables display specific requirements on the data, its characteristics and its errors (Table 1, Table 3 and Table 5), and requirements on the data format and associated metadata (Table 2, Table 4 and Table 6).



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3.2 Total ozone data product

Table 1. Product requirements for total ozone column data. Achievable and future target requirements are given, separated by a '-'.(Adapted from URD version 1.0, 2011)

		Geographical Zone		ne
Quantity	Driving Research topic	Tropics	Mid-	Polar
			latitudes	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)
Total uncertainty	Evolution of the ozone layer (radiative forcing)	2% (7 DU)	2% (7 DU)	2% (7 DU)
Total uncertainty Seasonal cycle and interannual variability; Short-term variability		3% (10 DU)	3% (10 DU)	3% (10 DU)
Stability (after corrections)	Evolution of the ozone layer (1980-2010 trend detection; radiative forcing)	1 – 3 % / decade	1 – 3 % / decade	1 – 3 % / decade

 Table 2. Data format and metadata requirements for total ozone. (From URD version 1.0, 2011)

Data feature	Requirement
Data format	netCDF [RD18]
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
Visualisation Basic browsable archive visualisation (daily global	
	local/latitudinal time series of monthly means)



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3.3 Ozone profile data product from nadir-viewing instruments

Table 3. 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 '-'.(From URD version 1.0, 2011)

		Height range		
Quantity	Driving Research topic	Troposphere	UT/LS	Middle
				Atmosphere
Horizontal	Regional differences in	100 – 200 km	100 – 200 km	100 - 200 km
resolution	evolution of the ozone layer			
	and tropospheric ozone			
	burden (radiative forcing);			
	Seasonal cycle and			
	interannual variability;			
	Short-term variability			
Vertical	Height dependence of	6 km –	3-6 km	3 - 10 km
resolution	evolution of the ozone layer	Tropospheric		
	and the tropospheric ozone	column		
	burden (radiative forcing);			
	Seasonal cycle and			
	interannual variability; Short-term variability			
Observation	Evolution of the ozone	3 days	3 days	3 days
frequency	layer and the tropospheric	3 days	3 days	3 days
rrequency	ozone burden (radiative			
	forcing); Seasonal cycle			
	and interannual variability;			
	Short-term variability			
Time period	Evolution of the ozone	(1980-2010) -	(1980-2010) –	(1980-2010) -
1	layer and tropospheric	(1996-2010)	(1996-2010)	(1996-2010)
	ozone burden (radiative			
	forcing)			
Total uncertainty	Evolution of the ozone	10 %	8 %	8 %
	layer and tropospheric			
	ozone burden (radiative			
	forcing)			
Total uncertainty	Seasonal cycle and	20 %	15 %	15 %
	interannual variability;			
G 1 111	Short-term variability	4 00//1	4 20//1	1 20//
Stability	Evolution of the ozone	1-3% / decade	1-3% / decade	1 – 3 % /
	layer and tropospheric			decade
	ozone burden (radiative			
	forcing); trends			



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Table 4. Data format and metadata requirements for nadir-based ozone profiles. (From URD version 1.0, 2011)

Data feature	Requirement	
Data format	netCDF [RD18]	
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	
Visualisation	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)	



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3.4 Ozone profile data product from limb-viewing instruments

Table 5. Product requirements for limb-based ozone profiles. 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. (Adapted from URD version 1.0, 2010)

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

Table 6. Data format and metadata requirements for limb-based ozone profile requirements. (URD v1.0, 2010)

Data feature	Requirement	
Data format	NetCDF [RD18]	
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	
Visualisation	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)	



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4 ECV Product Evaluation Protocol

4.1 Foreword

This chapter starts with the general principles applicable to the validation of the three ozone ECVs. It gets on with the specific characteristics applicable for each of the three ozone ECV products. As a baseline, generic principles and means for validation shall prevail over specific provisions whenever possible, in order to enable a standardised approach. This chapter applies to the full validation of the final ECV products. Unless stated differently, it also applies to more focused validation activities foreseen in interim and Round Robin exercises as defined in the next chapter.

4.2 Generic principles applicable to all ECVs

4.2.1 Core requirements of the GEOSS data quality strategy (QA4EO)

The Quality Assurance Framework for Earth Observation (QA4EO) [RD16] establishes general principles of the data quality strategy for the GEOSS. The core requirement of QA4EO is that all data and derived products have associated with them a documented and fully traceable quality indicator (QI). A quality indicator shall provide sufficient information to allow all users to readily evaluate the "fitness for purpose" of the data or derived product. A quality indicator shall be based on a documented and quantifiable assessment of evidence demonstrating the level of traceability to internationally agreed (where possible SI) reference standards.

4.2.2 Principles of the validation of atmospheric data

The validation of an atmospheric ozone data product can be seen as a science-driven verification process, the aim of which being to verify that the data produced do respond to predefined quality requirements and information content requirements. Validation generally involves the assessment of the closeness of the data to the geophysical reality, and of its sources of uncertainty, over the spatial and temporal domains of relevance as defined in URD. Uncertainty estimates can include, but are not restricted to, estimates of the bias and precision of the data with respect to reference data, and identification of the temporal and spatial domains over which those estimates are valid. Standard concepts of the classical metrology, like precision and repeatability, usually apply to atmospheric measurements. However, they can be of limited suitability for modelling results, for which more dedicated quality indicators shall be defined. It must be noted that international standardisation bodies insist on the fact that accuracy – defined as the closeness of agreement between a quantity value obtained by measurement and the true value of the measurand – is not a quantity and hence is not given a numerical quantity value [RD14].

4.2.3 Principles of the validation of an ECV product line

In a metrology-like approach of validation, the quality of data products must be evaluated (1) through assessment of uncertainties associated with the way the data product is measured or calculated, and (2) through confrontation with 'reference' measurements showing documented evidence of quality traceable to international standards, following community agreed practices. In the context of CCI, quality must be evaluated also through critical analysis of the suitability of the data products for the targeted applications (validation of actual usability).

Figure 2 presents an overview of the main validation tasks and quality control mechanisms to be applied over the life cycle of every ECV production.



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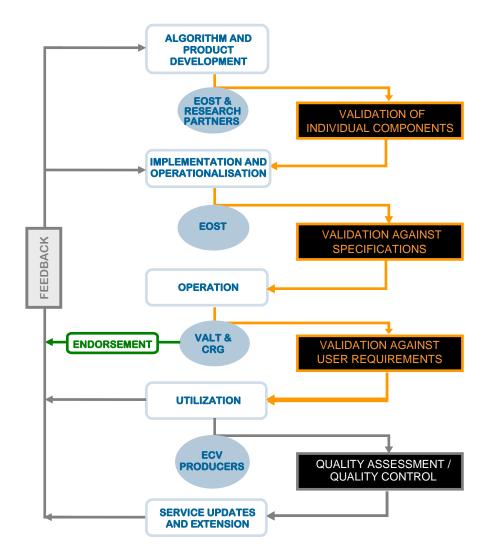


Figure 2 Validation tasks, quality control mechanisms and feedback loops over the life cycle of an ozone ECV production line.

From top to bottom, the box chart shows the timeline for the evolution of an ECV production line (centre line blue square boxes) through phases from the build-up through operations to updates and its associated validation steps (right-hand line of orange square boxes). The high level appointment of responsibilities is outlined in the centre line (oval boxes), highlighting the respective role of research partners, of system developers and ECV producers (EOST), of validation teams (VALT) and climate research users (CRG), and of ECV producers in the general QA/QC loop. Major feedback loops are also highlighted, from those associated to operations feedback into improvements of algorithms and their operationalisation into ECV production lines, to the formal endorsement by CRG users. The latter step concludes officially the build-up of an operational service. The following sections describe the major validation tasks in more details.



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4.2.4 Confrontation with independent reference data

4.2.4.1 Generalities

The performance of calibration procedures, retrieval algorithms and merging systems, and the quality of the resulting ECV products will be assessed by comparison with reference measurements providing the atmospheric "truth". A key aspect of any comparison for validation purposes is the selection of the reference data sets. The quality, traceability and suitability of the latter are essential to allow proper, unbiased and independent validation. Reference measurements must be well documented and procedures must exist to ensure adequate quality control on the long term, as it is the case e.g. within international ground-based networks.

Where and when reference observations are available, they constitute the preferred source of validation data, superseding the use of modelling results as validation data. When suitable measurements are not available, validation of data might also involve comparisons with "reference" model data sets. Models are of valuable use to extend measurement based validation to the global domain and to a better sampling of temporal and spatial features, to verify data products under atmospheric states and scenarios not accessible to the measurement, to assess comparison errors due to temporal and spatial mismatch and sampling differences, and to identify inconsistencies in the data sets under investigation. However models, including data assimilation systems must always be used with circumspection in validation as they are based on our current understanding of the atmosphere and they can suffer from many limitations and uncertainties.

4.2.4.2 Reference measurements from GAW ground-based networks

Ground-based reference measurements of the total column and vertical distribution of ozone are performed by networks of instruments contributing to WMO's Global Atmosphere Watch programme (GAW) [RD20]. Data sets suitable for the validation analysis of ECV products are collected from complementary instruments archiving routinely their data to the World Ozone and Ultraviolet Radiation Data Centre (WOUDC) and the Data Host Facility (DHF) of the Network for the Detection of Atmospheric Composition Change (NDACC). Individual details are given in the Data Access Requirement Document (DARD) [RD4]. Access conditions and pricing as applicable to the two data archives are regulated by data protocols available on the web portals of the data archives (http://woudc.org and http://ndacc.org, respectively).

It should be pointed out that the Ozone_CCI project does not foresee the production of any independent validation measurements. It needs to rely completely on observations and results provided by existing monitoring networks and ongoing/planned research projects as described in the DARD. High-level impetus through ESA, CEOS, the EC, space agencies and national agencies funding instrument operation as part of networks, is also required, in particular to ensure data provision suitable for sustainable validation activities of the future operational ECV production.

4.2.4.3 Error budget of a data comparison

A major objective of quantitative comparisons with reference measurements and modelling results of documented quality is to estimate uncertainties of the validated data product and to check the accuracy of its theoretical uncertainty estimates. But in fact the systematic and random discrepancies between the validated data set and the validation data set combine uncertainties associated with each individual system, plus uncertainties associated with the selection of data and the methodology of comparison. Discrepancies include the effect of the following comparison uncertainties:

(1) Comparison uncertainties associated with the difference in sampling of atmospheric variability and structures: e.g. geographical mismatch, diurnal cycle effects in the upper stratosphere and mesosphere (USM), assumptions related to the area of representativeness.



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(2) Comparison uncertainties associated with the difference in smoothing of atmospheric variability and structures: e.g., balloon-based in situ measurement at about 150m resolution by an electrochemical cell, compared with GOME ground pixels of 40 x 320 km² and vertical resolution of 3-8km.

As far as possible, most comparison uncertainties will be reduced by a cautious design of the selection of data sets to be compared, and by considering that a multivariate analysis of the comparison results taking into account the specifics of the data being compared (modelling data or remote sensing data, atmospheric variability and gradients etc.) might be required and preferred over entirely statistical approaches. For traceability purposes it is essential to document for each validation exercise the selection method applied to the data sets (temporal and spatial co-location criteria, how differences in vertical and horizontal smoothing are handled etc.)

Although essential if a rigorous metrological approach is to be adopted, the derivation of a complete error budget for each comparison is still a matter of research at the time being and it falls partly beyond the scope of the Ozone_CCI project. Validation teams as well as EOST are aware that neglecting uncertainties linked to the comparison method can spoil the value of the comparison and yield erroneous conclusions on the quality of the compared data product. This awareness must be transmitted to the reader of Ozone_CCI Validation Reports for a proper use of the validation results and, in fine, of the ozone ECV data records. When misinterpretation is possible, common statements like "the discrepancy between the two data sets ranges within their individual error bars" will be suitably annexed with a provision on the – really calculated or simply expected – contribution of the selection and comparison methods to this discrepancy. Provisions like "temporal and spatial mismatches exist but their contribution to the discrepancy between the two data sets has not been assessed; nevertheless this contribution is assumed to be small..." or "the selection method has been optimised to reduce apparent discrepancies between the data products, that would be generated actually by temporal and spatial mismatch and by differences in smoothing of atmospheric variability" are acceptable examples.

4.2.4.4 Information content

A key aspect in the validation of usability (the verification of "fitness for purpose" of a data product) is the characterisation of the information content of the data product. The retrieval of geophysical quantities from remote sounding measurements usually uses a set of a priori constraints, e.g. in the form of an assumed range of atmospheric profile shape around a first guess. Such constraints mix somehow in the retrieved quantities with the information really contributed by the measurement. When a climatology is used in the retrieval, e.g. at altitudes where the measurement is not or less sensitive due to optically thick clouds or too low signal-to-noise ratios, it is important to understand what, in the final product, comes from the climatology and what comes really from the measurement. That kind of validation of the information content can rely on a combination of (1) comparisons with independent reference data sets, especially during events not considered in the climatology, (2) the study of deviations of the retrieved product from the a priori constraints, and (3) sensitivity analysis of the retrieval, e.g. based on a study of the associated averaging kernels and their eigenvectors. E.g., plotting as a function of altitude the sum of the rows of the averaging kernel matrix associated with a retrieval shows at which altitudes the measurement offers sensitivity to atmospheric concentrations. Similarly, the real information content of the reference measurement itself should be known prior to performing a comparison. Information content studies might be an important aspect of the validation of model runs that have been initialised by climatology or by the output of another model, or that are constrained by a priori boundary conditions. They can also be of relevance in the assessment of data assimilation results when observations outside of a predetermined range are rejected as outliers by the data ingestion scheme, producing in the system a zero information zone similar to the dead band or neutral zone used in voltage regulators and controllers to avoid unwanted oscillations and disruptions. Information content studies are also essential in understanding data products generated by data merging and ensemble approaches.

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4.2.5 Validation of individual components

ECV line components are the individual processing blocks by which ECV data products are generated in their interim or final version. For complex processing chains international standards require to validate or at least verify the good performance of every component and the accuracy of its output. Limiting validation to the final data product only is not sufficient. The validation of intermediate data products is highly desirable to avoid e.g. that the apparently good behaviour of the final data product at the end of the chain hides large compensating errors affecting separate components of the data retrieval. Testing is one of many verification activities intended to confirm that software development output meets its input requirements. Other verification activities include various static and dynamic analyses, code and document inspections, walkthroughs, and other techniques.

4.2.6 Validation against service specifications

Service specifications are outlined in several documents like Product Specification Documents (PSD) and Algorithm Theoretical Basis Documents (ATBD). Verification of every product specification is out of scope of the project. The focus will be on service specifications having clear links with climate research user requirements expressed in the URD [RD6] or deduced from the known use of the data.

4.2.7 Validation against user requirements

User requirements are defined in the URD [RD6], on which summary tables reproduced in Section 3 are based. Products need to be validated against these official user requirements. Compliance with requirements on observation frequency is straightforward to verify. Compliance with requirements on bias and precision can be verified by classical comparisons yielding bias and precision estimates, taking into account comparison error terms. Compliance with requirements on spatial resolution and spatial sampling need visualisation of the data and analysis of information content (e.g., calculation of centroids and Backus-Gilbert spread and use of cross-correlation techniques). Compliance with more specific requirements, e.g. in terms of actual geographical coverage and of point-to-zone representativeness, may need the use of statistical methods based on global model results. In addition to quality checks on the part of the validation teams and the ECV producers and on the basis of known user requirements, user feedbacks provide valuable input for the assessment of the ECV compliance in terms of the accuracy (bias, precision or other estimates) and effective usability of the data product.

4.2.8 Quality control of operational ECV production

Continuous monitoring of each production line component (e.g. retrieval, modelling, assimilation processes etc.) within the entire process chain is required (online validation). This comprises monitoring of the operational workflow as well as a permanent quality check of the resulting products. Process failures and data losses have to be documented. Generally, the focus of offline services will be put more on product accuracy, whereas near-real time services (NRT) will be also assessed on the basis of their operational functioning (delay time, loss rate etc.) In particular, NRT services require access to online available independent measurements from operational networks for automatic validation.

4.2.9 Validation of ECV product updates

Whenever a major upgrade of an ECV production line occurs (switch to a new sensor, improved retrieval algorithm, updated spectroscopic databases, higher grid resolution...), steps 1 to 3 of the validation in the build-up phase have to be performed and documented: validation of individual components, against service specifications, and against user requirements. The focus must be on the verification of expected product changes. A verification of the entire processing chain might be required as well. A record of successive updates and corresponding validations should be maintained and made publicly available by the ECV producer. The ECV producer has to exercise judgement as to the extent of validation needed for a particular service revision, as this will depend on the nature and importance of changes being made. It is also not feasible to test all changes in advance: e.g., sudden degradation of a satellite instrument may necessitate emergency removal of that source from a near-real-time production process.

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4.3 Validation specifics by ECV

4.3.1 Total ozone data product

4.3.1.1 Validation requirements

Validation studies and resulting documentation will address the following targets:

- o Time series of ECV total ozone data and of the main measurement and retrieval parameters with potential impact on the data quality (AMF, cloud properties, SZA...) should be visualised, at least in selected latitude zones and at a few representative ground-based stations. Any obvious quality issue like the frequent occurrence of outliers and unrealistic values should be detected, documented and filtered out appropriately before performing quantitative comparisons.
- o The error bar on ECV total ozone data (δ TOC) shall be assessed and expressed as the percent relative difference with respect to correlative measurements of reference.
- Statistical estimators of the difference like the bias and the spread shall be calculated over different time periods and over different ranges of relevant parameters as listed below. In case of frequent occurrence of outliers, median and interpercentile values shall be preferred over mean and standard deviation values as they reduce the influence of outliers. Calculation of mean values and associated standard deviation is nevertheless encouraged. In case of doubt, histograms of the relative difference might be helpful in determining the validity of statistical estimators.
- o In the treatment of statistics, care will be given to decouple as far as possible the different sources of ECV uncertainty and avoid misleading cancellation of mutually compensating errors.
- Decadal stability of the bias and spread shall be assessed and expressed in %/decade.
- o Based on at least bi-weekly sampling of the time series over at least five years, shorter term stability of the bias and spread shall be assessed, including annual cycle, interannual variability and shorter term variability of the bias.
- o The dependence of the ECV data quality on main measurement and retrieval parameters like the solar zenith angle, ozone column amount, latitude, and cloud parameters (fractional cloud cover, cloud top height and albedo, etc. as appropriate) shall be investigated.
- O Studies shall be carried out at least in three geographical zones, in both hemispheres: tropics, middle latitudes and polar areas. Higher meridian and regional sampling is encouraged where possible.

4.3.1.2 Validation data sources

As described in DARD [RD4], the following measurement data sets will be used as reference for validation studies and/or for cross-comparison studies:

- Ground-based ozone column measurements by Dobson and Brewer ultraviolet spectrophotometers, up to 80° SZA for Brewers MK-III and MK-IV and 70-75° of SZA for Dobsons and other Brewers.
- o Ground-based ozone column measurements by UV-visible DOAS spectrometers.
- o Satellite ozone column measurements by EP-TOMS and EOS-Aura OMI (both OMI-TOMS and OMI-DOAS algorithms).
- Where appropriate, comparisons with satellite ozone column measurements by GOME, SCIAMACHY and GOME-2 retrieved by alternative processing facilities and algorithms is encouraged.



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4.3.2 Ozone profile data product from nadir-viewing instruments

4.3.2.1 Validation requirements

Validation studies and resulting documentation will address the following targets:

- o Time series of ECV ozone profile data and of the main measurement and retrieval parameters with potential impact on the data quality (SZA, cloud properties...) should be visualised, at least in selected latitude zones and at a few representative ground-based stations. Any obvious quality issue like the frequent occurrence of outliers and unrealistic values should be detected, documented and filtered out appropriately before performing quantitative comparisons.
- o Information content issues like the long-term degradation of the Degree of Freedom of the System (DFS) will be studied based on the analysis of vertical averaging kernels and, where relevant, of deviations from the a priori profile.
- o Studies shall address ozone in the troposphere, in the UT/LS and in the middle atmosphere.
- o The error bar on ozone concentration/partial column shall be assessed and expressed as the percent relative difference with respect to correlative measurements of reference. Uncertainties on height registration shall be expressed as the deviation of the centroid from the nominal retrieval altitude. Dependences on time, SZA, latitude... should be identified. VALT, EOST-2 and CRG should agree on a common definition of the tropopause, to be used consistently by all.
- Statistical estimators of the difference like the bias and the spread shall be calculated over different time periods and over different ranges of relevant parameters as listed below. In case of frequent occurrence of outliers, median and interpercentile values shall be preferred over mean and standard deviation values as they reduce the influence of outliers. Calculation of mean values and associated standard deviation is nevertheless encouraged. In case of doubt, histograms of the relative difference might be helpful in determining the validity of statistical estimators.
- o In the treatment of statistics, care will be given to decouple as far as possible the different sources of ECV uncertainty and avoid misleading cancellation of mutually compensating errors.
- o Decadal stability of the bias and spread shall be assessed and expressed in %/decade.
- o Based on at least bi-weekly sampling of the time series over at least five years, shorter term stability of the bias and spread shall be assessed, including annual cycle, interannual variability and shorter term variability of the bias.
- o The dependence of the ECV data quality on main measurement and retrieval parameters like the solar zenith angle, ozone slant column amount and latitude shall be investigated.
- o Studies shall be carried out at least in three geographical zones: tropics, middle latitudes and polar areas. Higher meridian and regional sampling is encouraged where possible.

4.3.2.2 Validation data sources

As described in DARD [RD4], the following measurement data sets will be used as reference for validation studies and/or for cross-comparison studies:

- o Ground-based ozone profile measurements by balloon-borne ozonesondes.
- o Ground-based ozone profile measurements by stratospheric ozone lidars.
- Optionally, where appropriate, satellite measurements of stratospheric ozone profile at higher vertical resolution by ERBS SAGE-II, UARS HALOE and EOS-Aura MLS.

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4.3.3 Ozone profile data product from limb-viewing instruments

4.3.3.1 Validation requirements

Validation studies and resulting documentation will address the following targets:

- o Time series of ECV ozone profile data and of the main measurement and retrieval parameters with potential impact on the data quality (e.g. SZA for SCIAMACHY) should be visualised, at least in selected latitude zones and at a few representative ground-based stations. Any obvious quality issue like the frequent occurrence of outliers and unrealistic values should be detected, documented and filtered out appropriately before performing quantitative comparisons.
- o Potential information content issues like long-term changes of the resolution will be studied based on the analysis of vertical averaging kernels.
- o Studies shall address at least ozone in the lower stratosphere and in the middle atmosphere.
- o The error bar on ozone profile data shall be assessed and expressed as the percent relative ozone difference with respect to correlative measurements of reference.
- o Where possible the theoretical error bar on altitude will be verified by the comparisons. Several methods might be considered: analysis of centroids, cross-correlation between satellite and reference profiles, and chi square. Depending on the satellite sensor and retrieval technique, the height registration uncertainty can vary with several parameters like time, SZA, latitude...
- Statistical estimators of the difference like the bias and the spread shall be calculated over different time periods and over different ranges of relevant parameters as listed below. In case of frequent occurrence of outliers, median and interpercentile values shall be preferred over mean and standard deviation values as they reduce the influence of outliers. Calculation of mean values and associated standard deviation is nevertheless encouraged. In case of doubt, histograms of the relative difference might be helpful in determining the validity of statistical estimators.
- o In the treatment of statistics, care will be given to decouple as far as possible the different sources of ECV uncertainty and avoid misleading cancellation of mutually compensating errors.
- o Decadal stability of the bias and spread shall be assessed and expressed in %/decade.
- Based on at least bi-weekly sampling of the time series over at least five years, shorter term stability of the bias and spread shall be assessed, including annual cycle, interannual variability and shorter term variability of the bias.
- o The dependence of the ECV data quality on measurement and retrieval parameters, like e.g. SZA for SCIAMACHY and star brightness for GOMOS, and latitude for all, shall be investigated.
- o Studies shall be carried out at least in three geographical zones: tropics, middle latitudes and polar areas. Higher meridian and regional sampling is encouraged where possible.

4.3.3.2 Validation data sources

As described in DARD [RD4], the following measurement data sets will be used as reference for validation studies and/or for cross-comparison studies:

- o Ground-based ozone profile measurements by balloon-borne ozonesondes.
- o Ground-based ozone profile measurements by stratospheric ozone lidars.
- o Satellite measurements of stratospheric ozone profile by ERBS SAGE-II, UARS HALOE and EOS-Aura MLS.
- Optionally, satellite ozone profile measurements at lower resolution by a series of SBUV/2 on NOAA-9/11/14/16/17/18 operational polar satellites, and by EOS-Aura OMI.



5 Round Robin and Interim Evaluation Protocols

5.1 Scope and generalities

Prior to the generation of final ECV data products and their full validation – as described in Section 4 – algorithm and product developments within the Ozone_cci project require different interim evaluation activities, for which the present protocol defines principles and guidelines. When different algorithms are available and in competition, the Round Robin Evaluation Protocol specifies evaluation procedures and criteria supporting the selection of the 'best' retrieval algorithm to generate the final ECV data product (for MIPAS limb ozone profile data), or the 'best' parts of retrieval algorithms to be assembled for the generation of the final ECV data product (for nadir ozone profile data). The Interim Evaluation Protocol defines the set of validation tasks to be carried out when an algorithm has been selected, before it is applied for the reprocessing of the entire level-1 data record (for GOMOS and SCIAMACHY limb ozone profile data). The Interim Evaluation Protocol has also to be applied when an algorithm selected for a given level-1 data set is transferred to the analysis of another level-1 data set, either from the same satellite instrument or from another one (for total ozone data).

Interim and Round Robin evaluation activities consist of dedicated subsets of the full ECV evaluation, carried out on subsets of the available satellite and correlative data records. Nevertheless, the general principles and requirements described in the previous section remain the cornerstone of all interim evaluation activities. In particular, activities and reporting shall comply with all articles of Section 4.2 and relevant articles of Section 4.3. Care shall be given to produce accurate documentation of the algorithm, of the data, of the evaluation process and of the evaluation results. Selection criteria in the case of Round Robin exercises, and quality indicators in the case of interim evaluations, will be based on the availability and appropriateness of the algorithm, data and documentation (including metadata):

- o <u>Retrieval algorithm</u>: Are the retrieval concept and implementation accepted by the community, verified through algorithm inter-comparison exercises, sanctioned by peer-reviewed documents, and up-to-date? Is the algorithm description available (e.g. through ATBD) and complete, with a sufficient level of detail to judge its validity and its potential capabilities in the CCI context? Are there particular features revealed by algorithm verifications and inter-comparisons, like e.g. negative values, biases, vertical oscillations, incoherent geographical structures?
- <u>Level-2 data</u>: Is the data available? In parts only or the complete data record? Publicly or with restricted/controlled access? Is the data description sound and complete (e.g. PSD)? Is there a need for data extraction and reading routines and are they available? Is the processing chain well identified: name and reference of the processors, location, version of level-1 data, and version of level-1-to-2 processing? Is the data accompanied by relevant error bars/uncertainty estimates calculated with community agreed methods and associated metadata, including diagnostic quantities for every measurement: e.g., error covariance and averaging kernel matrices, a priori profile, and parameters required for data filtering like e.g. star brightness, occultation obliquity and solar zenith angle?
- Ouality assurance: Has the data been validated? If yes, how and how far? With respect to which correlative data of reference, traceable to international standards? Against which user requirements? Is the validation process well described, accompanied by relevant validation metadata, and compliant with community agreed practices, especially regarding data manipulations (e.g. re-gridding and smoothing operations)? Are the validation results well documented and leading to clear quality indicators? Is the terminology unambiguous and compliant with recommended standards? Apart from comparison results, are there particular features affecting the quality of the data, like e.g. negative values, biases, vertical oscillations, incoherent geographical structures? Does the published use of the data demonstrate its fitness for purpose in the context of the Ozone cci project?



5.2 Interim evaluation of total ozone data products

The baseline total ozone algorithm for the Ozone_cci project is the so-called GODFIT direct-fitting algorithm. It is currently implemented in version 5.0 of the GOME Data Processor (GDP) and transferred to SCIAMACHY and GOME-2 as part of the project. Alternative (non-CCI) GOME and SCIAMACHY total ozone data products and algorithms, as well as OMI total ozone data available through the TEMIS and TOMS web portals, will be used for comparison and assessment purposes.

As a baseline, validation tasks and resulting documentation will address the targets outlined in Section 4.3.3.1 and answer explicitly the questions listed in Section 5.1, with the objective to verify that the algorithm transfer, associated evaluation and available documentation meet the Ozone_cci requirements. Examples of suitable interim evaluations can be found in delta validation reports for GDP 3.0 ([RD28]) and 4.0 (RD27). Comparisons can be limited to appropriate subsets of correlative data records and ground-based stations, the main objective being to verify that the transfer of the GODFIT direct-fitting algorithm to SCIAMACHY and GOME-2 performs according to the expectations. Special care shall be given to detect negative and other unrealistic values, biases, incoherent geographical patterns, oscillations, enhanced noise... in the total ozone data as well as in the retrieval parameters (slant column, AMF, cloud properties...) Tasks should include the visualisation both of time series and of global maps.

5.3 Round Robin evaluation of ozone profile data products from nadir-viewing instruments

No firm algorithm baseline exists for ozone profile data processing from nadir measurements. Two existing scientific algorithms developed at KNMI (OPERA) and at RAL, and applicable to all sensors, will be intercompared and characterised in a Round Robin exercise. Results of this evaluation will support the determination of the new Ozone-cci nadir profile algorithm baseline, which will be a combined RAL/OPERA algorithm.

As a baseline, validation tasks and resulting documentation will address the targets outlined in Section 4.3.2.1. Depending on the needs, comparisons can be limited to appropriate subsets of correlative data records and ground-based stations. Special care shall be given to the detection of negative and other unrealistic values, biases, incoherent geographical patterns, oscillations, enhanced noise... in the ozone profile data as well as in the retrieval parameters and diagnostics (averaging kernels...) Tasks should include the visualisation both of time series and of global maps. The quality and information content of ozone profile retrievals being strongly dependent on the accuracy and stability of the level-1 radiance data, particular efforts will be dedicated to characterising the accuracy, long-term stability and cross-consistency of the level-2 ozone profile data from each sensor, with particular attention to degradation issues. Characterisation will include the analysis of diagnostics derived form the averaging kernels, like DFS, Backus Gilbert spread and centroids, including their variations with time, latitude and ozone slant column. Ground-based validation can be performed on partial columns at the resolution (1) specified by EOST-2, (2) derived from the AK analysis (if different), (3) of the retrieval by means of a priori and AK manipulations, (4) if broader than the retrieval resolution, at the resolution requested by users.

5.4 Interim evaluation of GOMOS limb ozone profile data

The baseline ozone profile algorithm for GOMOS limb measurements of stellar occultation has been determined as part of the Envisat GOMOS Quality Working Group. No further algorithm development is foreseen in the framework of the Ozone_cci project. Detailed evaluation of the current version GOPR 6.0cf is performed within the ESA-funded Multi-TASTE and VALID projects. Results reported by these projects will undergo verification of compliance with the targets outlined in Section 4.3.3.1 and with the specific questions listed in Section 5.1. In case of severe non compliance with Ozone_cci requirements, complementary validation tasks might be undertaken in the framework of the Ozone_cci project.



5.5 Round Robin evaluation of MIPAS limb ozone profile data

MIPAS level-2 data are processed by ESA/DLR plus by several scientific institutions, namely: IFAC Florence, IMK/IAA, ISAC Bologna, Leicester University, and Oxford University. They will participate in a Round Robin exercise, which will support the selection of the 'best' processor for generating the ECV limb ozone profile data from MIPAS.

All MIPAS ozone retrieval processors rely on level-1b data provided by ESA. Delivery of level-1b version (IPF) 5 has started in January 2010 – from January 2010 on only level-1b version 5 is available; before January 2010, the level-1b data were 4.61/62 for data acquired at Full Resolution (FR) and 4.67 for data acquired at Reduced resolution (RR); reprocessing of older data with IPF V5 is ongoing. The level-2 algorithms differ considerably: IFAC Florence uses ORM which is the prototype code of the ESA/DLR processor (with further functionalities); IMK/IAA uses a Tikhonov-constrained 1D global fit (KOPRA/RCP); Oxford and Leicester use optimal estimation (MORSE); ISAC Bologna uses a 2D-global fit approach (GEOFIT). The level-2 data sets of the different institutions differ by spatial/geographical representation, temporal and spatial coverage, data and error characterisation, availability of averaging kernels, and by values. Main characteristics of the data are given in DARD ([RD4]).

As a baseline, validation tasks and resulting documentation will address the targets outlined in Section 4.3.3.1 and answer explicitly the questions listed in Section 5.1. Depending on the needs, comparisons can be limited to appropriate subsets of correlative data records and ground-based stations. Special care shall be given to the detection of negative and other unrealistic values, biases, incoherent geographical patterns, oscillations, enhanced noise... in the ozone profile data as well as in the retrieval parameters and diagnostics (averaging kernels...) Tasks should include the visualisation both of time series and of global maps produced on regular intervals. All datasets participating in the Round Robin will cover a period of two consecutive years, chosen by the consortium to be years 2007 and 2008. Additional data sets prior to 2005 might be envisaged in order to cover both the original (FR, until 2005) and the optimised (RR, after 2005) resolution mode of MIPAS.

5.6 Interim evaluation of SCIAMACHY limb ozone profile data

The SCIAMACHY level-2 version 2.3 data (current version) is produced by applying the SCIATRAN radiative transfer model and retrieval package to level 1-b data to retrieve the ozone limb vertical profile. The Ozone_cci project includes further optimisation of the retrieval software package and its application to the SCIAMACHY level-1 version 8 data set. The latter includes the most advanced degradation corrections.

As a baseline, validation tasks and resulting documentation will address the targets outlined in Section 4.3.3.1 and answer explicitly the questions listed in Section 5.1, with the objective to verify that the algorithm improvements and available documentation meet the Ozone cci requirements.



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6 Standards

6.1 Maintenance of datasets and reports

It is essential to ensure long-term archiving of ECV data products and their metadata, of validation results and of associated metadata on the validation process, all needed to qualify the stored products and guarantee their proper use in the future and by an always wider community. This is achieved by relying on operational archiving systems of the service providers and on the Ozone-cci web site.

I/O documentation and tools for the formats of end products are provided by the ECV producers. Formats are selected in agreement with the users (NetCDF [RD18] in the Ozone_cci project). Standards endorsed by European Corporation for Space Standardization (ECSS) are applied whenever possible to assure high quality software. However, given the large amount and complexity of existing codes, a reprogramming is not feasible.

6.2 Metadata and additional information

The principle of transparency is a prerequisite for interoperability and an essential part of good administration at all levels of governance. It means that important information is readily accessible and widely spread and communicated to all stakeholders. Beyond comparison results obtained as part of a geophysical validation process, important information covers evaluation from the point of view of the source, technical attributes, quality levels and use conditions, in order to be able to determine whether the data and service are fit for their particular purpose.

Some of this information may be readily available as metadata, but additional information should also be made available if requested to allow an assessment of fitness for purpose to be made. This is particularly important when the data is being used for a purpose which is different from that for which it was originally produced or collected.

Metadata, whether applying to a dataset or to a service, are necessary for users to:

- o Identify and locate the datasets or services they need ("discovery metadata").
- o Be aware of the general context through which the data was collected and made available (research project, programme, etc.), of possible access conditions and of applicable usage rules (such as acknowledgement or citation).
- o Retrieve and read the data (format metadata) or access the products provided.
- o Understand and interpret the data and their limitations (scientific metadata).
- o Seek further information or help if required (references, links, contact).

In order to fulfil what is expected from them, metadata should be:

- o Specific: achieving the level of detail required to an in-depth understanding.
- o Accurate: achieving a level of precision sufficient to avoid ambiguities "accurate" and "precise" here refer to qualities of the wording, not to data.
- Explicit: avoiding coded information, abbreviations and acronyms unless appropriate keys are provided.
- o Complete: covering all relevant information, with no omission.



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6.3 QA and validation metadata

To facilitate proper interpretation of the validation results, traceability of the validation process is essential. Therefore validation metadata, that is, brief but unambiguous documentation of the entire validation process leading to a validation graph or a comparison data file, should accompany any validation result reported in validation reports and on the project web site. Where validation results are provided in graphical format (e.g. in a .jpeg file), validation metadata can be provided in a legend placed on the graph itself or below; they can also be attached to the graphical file as a readme.file.text. Where validation results are provided in numerical format (e.g. in a ASCII or HDF file), validation metadata can be included in this numerical data file as a header or simply attached externally to the file.

The metadata on the validation process (also called correlative analysis) must provide a short, unambiguous description of the comparison manipulations undertaken to obtain the validation results. From this information one should be able to check if the validation process complies with agreed standards and best practices. The step-by-step description of the data manipulations should also allow proper interpretation of the comparison results and further investigation of the data quality.

Table 7 suggests the minimum information that should be available in the validation metadata to ensure traceability of the validation process. Ideally it should not duplicate information that is already available e.g. in the metadata accompanying the data under evaluation and the validation source.

 Table 7
 Suggested validation metadata

VALIDATION STEP / ITEM	DETAILS
High-level description of the content of validation results (graphic file or numerical data file)	Identification of the data being validated and of the reference data used as a validation source, date, basic description of the results being reported
Metadata on data under evaluation	Data processing and archiving centre, model or data processor version, input and initialisation data, native data format (e.g. number density or volume mixing ratio, versus altitude or pressure), data file name (at least file name convention)
Metadata on reference data used as a validation source	Data processing and archiving centre, instrument, responsible institute, model/data processor version, calibration version (input level-1 data), measured parameter, native data format
Traceability of validation process	Step-by-step description of the data manipulations: data selection, conversion of units, filtering based e.g. on flags or statistical tests, co-location criteria (vertical, horizontal and temporal), re-gridding, smoothing (vertical and horizontal, e.g. using a Gaussian, averaging kernels etc.), range of the comparisons (geographical, vertical, temporal), reference to an agreed reference practice
Format of validation results	Content of the numerical validation data file or description of the information displayed on the validation graph: units, relative or absolute difference, individual comparison pair or monthly mean, amount of comparison events, statistical estimators (mean/deviation or median/interpercentile)
Credit and responsibilities	Analysis carried out at institute X by validation scientist Y supported by data processing scientist Z, contact (email)



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6.4 Compliance with international standards

Interoperability is a driving concept of the GEOSS Implementation Plan in general and of CCI developments in particular. Elaborated in this context, the present document gives particular attention to international standardisation requirements formulated e.g. within high-level strategies like the QA4EO framework formalised by the Committee on Earth Observation Satellites (CEOS) and the Integrated Global Observation Strategy (IGOS) established by a list of international partners (including CEOS, GAW, GCOS, IGBP, UNEP, UNESCO, WCRP and WMO), and within European initiatives relevant to GMES. Further evolution is anticipated.

6.5 Compliance with INSPIRE

Particular attention must be given to the Directive 2007/2/EC of the European Parliament and of the Council of 14 March 2007, establishing an Infrastructure for Spatial Information in the European Community (INSPIRE) to support Community environmental policies, and policies or activities which may have an impact on the environment. Published in the Official Journal on the 25th of April 2007, the INSPIRE Directive entered into force on the 15th of May 2007. To ensure that the spatial data infrastructures of the Member States are compatible and usable in a Community and transboundary context, the Directive requires that common Implementing Rules (IR) are adopted in a number of specific areas (Metadata, Data Specifications, Network Services, Data and Service Sharing and Monitoring and Reporting). These IRs are adopted as Commission Decisions or Regulations, and are binding in their entirety. At the time of this issue of the Product Validation Plan, IRs have been negotiated and adopted for spatial data themes of Annex I, that is, Coordinate reference systems, Geographical grid systems, Geographical names, Administrative units, and five other themes, IRs for the spatial data themes under Annex II (Elevation, Land cover, Orthoimagery, and Geology) are being established. Data themes under Annex III have the more direct application to the Ozone cci project, among them: Atmospheric conditions, Environmental monitoring facilities, Statistical units, Human health and safety, Natural risk zones, Meteorological geographic features. For Annex III the Thematic Woking Group on Atmospheric Conditions and Meteorological Geographical Features has just issued the draft Data Specifications. The testing phase started in June 2011 and will last until October 2011. Active participation to this testing phase is beyond the scope of the Ozone cci project. The GMES Atmospheric Service projects MACC (core services) and PASODOBLE (air quality services) contribute to this testing phase.



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7 Compliance with ESA CCI guidelines

This section review the compliance of this PVP with requirements provided in the *ESA Climate Change Initiative /CCI project guidelines/* regarding CCI validation tasks in general (Table 8), Specific requirements in Annex B for the Ozone ECV (Ozone_cci) (Table 9), and Round-Robin comparison and selection in particular (Table 10).

Table 8 *General validation requirements for the CCI projects.*

	REQUIREMENT	COMPLIANCE	REMARKS
V-1	All CCI projects should use the definition of validation approved by the CEOS WGCV.	Full	Applicable terms and definitions are listed in the following section.
V-2	All CCI project Product Validation Plans (PVP) shall adhere to the above three requirements regarding independence.	Full	
V-3	The CCI teams shall use established, community accepted, traceable validation protocols where they exist. If such protocols do not exist then CCI project may adapt existing protocols if appropriate and in any event shall offer their final protocol for future community acceptance.	Full	Large parts of this PVP are adaptations of the GSE PROMOTE Validation Protocol, which is officially endorsed by ESA, ozone data producers and users. Ozone specifics of this PVP have been published in the peer-reviewed literature (see Reference Documents).
V-4	Each CCI project shall select appropriate validation data to ensure that an adequate level of validation (confidence) is applied to all output products. The level of validation (confidence) should be indicated in the output product.	Full	Appropriate validation data for the Ozone_cci project are described in the Data Access Requirement Document (DARD) and further mentioned in this PVP.
V-5	The CCI programme should hold a dedicated session (or workshop) on common validation infrastructure during (or prior to) the next co-location meeting.	Not applicable	Common validation infrastructures with first order functions – like GECA – are still under development. The development of common infrastructures meeting the high level requirements of climate research falls beyond the objectives and capabilities of the CCI project.
V-6	The PVP shall fully describe the validation process for each CCI project. An independent international review board of experts should be invited to review the PVP of each project team. Each CCI project should involve experts from the CMUG throughout their validation activities. A CCI product will be deemed to be validated once all steps of the validation process documented in the PVP have been completed and documented accordingly.	Full	A list of potential experts exists, who are members of key bodies like the IO ₃ C and SPARC.



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 Table 9 Specific requirements in Annex B of the Ozone ECV (Ozone_cci) Statement Of Work.

	REQUIREMENT	COMPLIANCE	REMARKS
TR8	• The contractor shall establish a plan for the validation of both the contributing satellite data (top of atmosphere radiances) and the burned area data product. This shall include:	Full	The validation of radiances is not part of the Ozone_cci project.
	o identifying the approaches,		
	o the key test sites,		
	o identification of existing validation data sets (see Section 11 as a starting point) and		
	o requirement for generation of new validation products to provide a comprehensive test.		
	• This shall be agreed by the engaged user community.	Full	
	• This plan is expected to evolve and shall be updated as the definition of the ozone ECV product consolidates and the understanding of algorithmic issues improves.	Full	
	• For each algorithm clear benchmark criteria shall be defined that will enable easy selection of the 'best' algorithms for processing implementation.	Full	
TR24	Validation shall be conducted independently of the groups charged with the product generation.	Partly	VALT consists of independent scientists with acknowledged expertise in atmospheric data validation. Satellite-to-satellite comparisons will be performed by EOST for practical reasons but also their procedures and results will be checked by VALT.
TR25	The final and intermediate ozone ECV products shall be validated against well characterised in-situ validation datasets (see Task 2). This shall be conducted on a sufficiently spatially and temporally comprehensive subset of satellite products and in-situ data to ensure that quantitative conclusions can be drawn from this exercise and requirements for further algorithm tuning or development steps can be established.	Full	See validation specifics by ECV in Section 4.3 and data description in DARD ([RD4])
TR26	The final and intermediate ozone ECV products shall be validated against other satellite ozone data (e.g. TOMS, TOMS/OMI, SBUV, MLS, SAGE, HALOE).	Full	See validation specifics by ECV in Section 4.3 and data description in DARD ([RD4])



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 Table 10 Requirements for the Round Robin algorithm inter-comparison and selection exercises.

	REQUIREMENT	COMPLIANCE	REMARKS
RR-1	The meaning of the 'best' algorithm and how to select it (evaluation protocol) has to be defined before the start of the Round Robin exercise. The definition of 'best' and the scope of the Round Robin exercise have to be specified in the Product Validation Plan (PVP).	Partly	This PVP only defines the scope and validation tasks of Round Robin exercises, which will support the selection of the 'best' algorithm. The definition of 'best' algorithm is out of scope of this document.
RR-2	The Round Robin should be made at the beginning of the project based on objective criteria. There should be one or more iterations to show algorithm improvement throughout the project. The most objective algorithm selection would be based on blind testing to avoid any bias.	Yes	
RR-3	Every CCI project has to perform a Round Robin exercise. In the exceptional case that a final algorithm has been pre-selected, component modules need to be tested also for this pre-selected algorithm. Furthermore, the pre-selection criteria should be in line with the CCI objectives.	Full	Interim and Round Robin evaluation exercises have been defined clearly and are in line with the CCI objectives.
RR-4	The same auxiliary and Level-1 data should be used in the processing, as well as the same reference data.	Full	
RR-5	The Round Robin results need to be open and the algorithm must be well-documented and public, but the actual code does not need to be public.	Full	The availability of appropriate documentation is a subsidiary selection criterion.
RR-6	The algorithm selection should be made by an independent team that is not directly involved in the algorithm development, although of course the members of that team should be experts. The selection shall be made based on a Round Robin evaluation protocol developed beforehand and providing objective criteria.		
RR-7	The development of new tools should only be considered when really needed and no good tools for the purpose are available.	Full	

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8 Terms and definitions

8.1 Terms and definitions

In Table 11 terms and definitions as recommended by CEOS WGCV and by standards development organisations of international recognition have been transcripted from reference documents [RD8] to [RD16]. In some cases terms and definitions peculiar to forecast systems are also proposed. They are expected to evolve as these organisations regularly update their standards and as further standardisation and harmonisation occur.

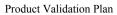
Table 11. Recommended terms and definitions

TERM	DEFINITION	SOURCE
accuracy	closeness of agreement between a quantity value obtained by measurement and the true value of the measurand; note that it is not a quantity and it is not given a numerical quantity value	VIM, GUM
area (volume) of representativeness	the area (volume) in which the concentration does not differ from the concentration at the station by more than a specific range	Larssen
	(1) systematic error of indication of a measuring system	VIM
bias	(2) estimate of a systematic measurement error	VIM
	(3) estimate of a systematic forecast error	GAS
	(1) the process of quantitatively defining the system responses to known, controlled signal inputs	CEOS
calibration	(2) operation that, under specified conditions, in a first step, establishes a relation between the quantity values with measurement uncertainties provided by measurement standards and corresponding indications with associated measurement uncertainties and, in a second step, uses this information to establish a relation for obtaining a measurement result from an indication	VIM
dead band (or neutral zone) maximum interval through which a value of a quantity being measured can be changed in both directions without producing a detectable change in the corresponding indication		VIM
measured quantity value, obtained by a given measurement procedu for which the probability of falsely claiming the absence of component, given a probability α of falsely claiming its presence		VIM
	(1) measured quantity value minus a reference quantity value	VIM
error	(2) difference of quantity value obtained by measurement and true value of the measurand(3) difference of forecast value and a, estimate of the true value	CEOS
establish	define, document and implement	CDRH
field-of-regard	an area of the object space scanned by the field-of-view of a scanning sensor	NIST
field-of-view	the solid angle from which the detector receives radiation	NIST
footprint	the area of a target encircled by the field-of-view of a detector of radiation, or irradiated by an active system	NIST
quantity that, in a direct measurement, does not affect the quantity that is actually measured, but affects the relation between the indication and the measurement result		VIM



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in situ measurement	(1) a direct measurement of the measurand in its original place (2) any sub-orbital measurement of the measurand	
measurand	quantity intended to be measured	VIM
metadata	data about the data; parameters that describe, characterise, and/or index the data	WMO
monitoring	(1) systematic evaluation over time of some quantity(2) by extension, evaluation over time of the performance of a system, of the occurrence of an event etc.	NIST
point-to-area (point- to-volume) representativeness	the probability that a point measurement lies within a specific range of area-average (volume-average) concentration value	Nappo
precision	closeness of agreement between quantity values obtained by replicate measurements of a quantity on the same or similar object under specified conditions	VIM
process validation	establishing documented evidence of a high degree of assurance that a specific process will consistently produce a product meeting its predetermined specifications and quality characteristics	CDRH
quality assessment (QA)	QA refers to the overall management of the processes involved in obtaining the data	CEOS
quality control (QC)	QC refers to the activities undertaken to check and optimise accuracy and precision of the data after its collection	CEOS
quality indicator (QI)	a means of providing a user of data or derived product with sufficient information to assess its suitability for a particular application. This information should be based on a quantitative assessment of its traceability to an agreed reference or measurement standard (ideally SI), but can be presented as a numeric or a text descriptor, provided the quantitative linkage is defined.	QA4EO
radiometric calibration	a determination of radiometric instrument performance in the spatial, spectral, and temporal domains in a series of measurements, in which its output is related to the true value of the measured radiometric quantity	NIST
random error	(1) component of measurement error that in replicate measurements varies in an unpredictable manner; note that random measurement error equals measurement error minus systematic measurement error (2) component of forecast error that varies in an unpredictable manner	VIM
relative standard uncertainty	standard measurement uncertainty divided by the absolute value of the measured quantity value	VIM
repeatability	measurement precision under set of conditions including the same measurement procedure, same operator, same measuring system, same operating conditions and same location, and replicated measurements over a short period of time	VIM
representativeness	the extent to which a set of measurements taken in a given space-time domain reflect the actual conditions in the same or different space-time domain taken on a scale appropriate for a specific application	Nappo
reproducibility	measurement precision under a set of conditions including different locations, operators, and measuring systems	VIM





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resolution	(1) the least angular/linear/temporal/spectral distance between two identical point sources of radiation that can be distinguished according to a given criterion (2) the least vertical/geographical/temporal distance between two identical atmospheric features that can be distinguished in a gridded numerical product or in time series of measurements; resolution is equal to or coarser than vertical/geographical/temporal sampling of the grid or the measurement time series	NIST
stability	ability of a measuring system to maintain its metrological characteristics constant with time	VIM
systematic error	component of measurement error that in replicate measurements remains constant or varies in a predictable manner	VIM
traceability	property of a measurement result relating the result to a stated metrological reference (free definition and not necessarily SI) through an unbroken chain of calibrations of a measuring system or comparisons, each contributing to the stated measurement uncertainty	VIM
tropopause	the region of the atmosphere where the environmental temperature lapse rate changes from positive (in the troposphere) to negative (in the stratosphere) the lowest level at which the lapse rate decreases to 2 °C/km or less, provided that the average lapse rate between this level and all higher levels within 2 km does not exceed 2 °C/km occasionally, a second tropopause may be found if the lapse rate above the first tropopause exceeds 3 °C/km	WMO
uncertainty	non-negative parameter that characterizes the dispersion of the quantity values that are being attributed to a measurand, based on the information used	VIM
	(1) the process of assessing, by independent means, the quality of the data products derived from the system outputs(2) verification where the specified requirements are adequate for an	CEOS
validation	intended use (3) the process of assessing, by independent means, the degree of correspondence between the value of the radiometric quantity derived from the output signal of a calibrated radiometric device and the actual value of this quantity.	VIM NIST
	(4) confirmation by examination and provision of objective evidence that specifications conform to user needs and intended uses, and that the particular requirements implemented through software can be consistently fulfilled	CDRH
verification	 (1) the provision of objective evidence that a given data product fulfils specified requirements; note that, when applicable, measurement uncertainty should be taken into consideration. (2) the provision of objective evidence that the design outputs of a particular phase of the software development life cycle meet all of the specified requirements for that phase 	VIM CDRH
vicarious calibration	a post-launch radiometric calibration of sensors performed with the use of natural or artificial sites or objects on the surface of the Earth (as opposed to calibration techniques using onboard standards such as lamps, blackbodies, solar diffuse reflecting panels etc.)	NIST



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8.2 Abbreviations and acronyms

Note of best practice: Using an acronym is acceptable if it has been defined the first time it appears in a document. The same applies to chemical abbreviations. In documents targeting a wide spectrum of potential readers, like user manuals and validation reports, it is recommended to avoid systematic use of acronyms and abbreviations except for those with frequent occurrence, and also those widely understood by the general public. For example, acronyms such as CFCs and ESA are acceptable. Acronyms such as ECSS and ICTT-QMF are not. Before using acronyms and abbreviations, authors should keep in mind that it is annoying and difficult – especially in Web-based documents unless the acronyms are available as hyperlinks – to turn over several pages in a document to verify the meaning.

AK Averaging Kernel

AMF Air Mass Factor, or optical enhancement factor

ATBD Algorithm Theoretical Basis Document
ATSR-2 Along Track Scanning Radiometer 2
AUTH Aristotle University of Thessaloniki
BIRA-IASB Belgian Institute for Space Aeronomy

CCI ESA's Climate Change Initiative programme
CDHR Center for Devices and Radiological Health
CEOS Committee on Earth Observation Satellites

CMDL Climate Monitoring and Diagnostics Laboratory (now ESRL)
CMUG Climate Modelling User Group of the CCI programme
CRG Climate Research Group of the Ozone cci project

DARD Data Access Requirement Document
DFS Degree of Freedom of the System

DHF Data Host Facility

DIAL Differential Absorption LIDAR DLR German Aerospace Centre

DOAS Differential Absorption Optical Spectroscopy

DU Dobson Unit – unit of vertical column density (2.69 10¹⁶ molec.cm⁻²)

EC European Commission ECC Electro Chemical Cell

ECSS European Corporation for Space Standardization

Envisat ESA's Environmental Satellite, launched March 1, 2002

EO Earth Observation

EOST Earth Observation Science Teams of the Ozone cci project

EPS EUMETSAT Polar System

ERS-2 ESA's Earth Remote Sensing satellite 2, launched April 21, 1995

ESA European Space Agency

ESRIN European Space Research Institute

ESRL Earth System Research Laboratory (formerly CMDL)

EUMETSAT European Organisation for the Exploitation of Meteorological Satellites

FMI-ARC Finnish Meteorological Institute – Arctic Research Centre

FTIR(S) Fourier Transform Infra Red Spectrometer

GAS GMES Atmospheric Service
GAW WMO's Global Atmosphere Watch
GCOS Global Climate Observing System

GDP GOME Data Processor
GEO Group on Earth Observation

GEOSS Global Earth Observation System of Systems
GMES Global Monitoring for Environment and Security

GOME Global Ozone Monitoring Experiment



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GOMOS Global Ozone Monitoring by Occultation of Stars

GSE GMES Service Element

GUM Guide to the expression of uncertainty in a measurement

HALOE Halogen Occultation Experiment

ICTT-QMF Inter-Commission Task Team on Quality Management Framework IGACO Integrated Global Atmospheric Chemistry Observation strategy

IGBP International Geosphere-Biosphere Project IGOS Integrated Global Observation Strategy

INSPIRE Infrastructure for Spatial Information in the European Community

IPF Instrument Processing facility

I/O tools Input/Output tools

IR INSPIRE Implementation Rule

ISO International Organization for Standardization

ISSI International Space Science Institute
JCGM Joint Committee for Guides in Metrology
KNMI Royal Dutch Meteorological Institute

lidar light detection and ranging

MCH Federal Office of Meteorology and Climatology (MeteoSwiss)

MetOp EUMETSAT's Meteorological Operational satellite

MIPAS Michelson Interferometer for Passive Atmospheric Sounding

MIPAS FR MIPAS operated at Full (nominal) Resolution MIPAS RR MIPAS operated at Reduced (optimised) Resolution

MLS Microwave Limb Sounder

Multi-TASTE Technical ASsistance To the multi-mission validation of Envisat and

Third Party Missions using spectrometers, radiometers and sondes Network for the Detection of Atmospheric Composition Change Network for the Detection of Stratospheric Change (now NDACC)

NOAA National Oceanic and Atmospheric Administration

NRT Near-real time

 O_3 ozone

NDACC

NDSC

O3M-SAF SAF on Ozone and Atmospheric Chemistry Monitoring

OE Optimal Estimation

OMI Ozone Monitoring Instrument OPERA Ozone Profile Retrieval Algorithm

PBL Planetary Boundary Layer

PROMOTE Protocol Monitoring for the GMES Service Element - Atmosphere

PSD Product Specification Document PTR Phillips-Tikhonov Regularisation

PVP Product Validation Plan

QA4EO Quality Assurance framework for Earth Observation

RAL Rutherford Appleton Laboratory

RMI Royal Meteorological Institute of Belgium

SAF Satellite Application Facility

SAGE Stratospheric Aerosol and Gas Experiment

SBUV Solar Backscatter Ultraviolet

SCIAMACHY SCanning Imaging Absorption spectroMeter for Atmospheric

CHartographY

SGP SCIAMACHY Ground Processor

SHADOZ Southern Hemisphere ADditional Ozonesondes

SZA Solar Zenith Angle

TEMIS Tropospheric Emission Monitoring Internet Service

TOC Total Ozone Column

TOMS Total Ozone Mapping Spectrometer



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TTOC Total Tropospheric Ozone Column

UCAM University of Cambridge

UARS Upper Atmosphere Research Satellite, launched September 15, 1991

UNEP United Nations Environment Programme

UNESCO United Nations Educational Scientific and Cultural Organization

URD User Requirement Document
USM Upper Stratosphere/Mesosphere

UT Upper Troposphere

UTLS Upper Troposphere/Lower Stratosphere
UVVIS DOAS UV-visible spectrometer (generic)
VALT Validation team of the Ozone_cci project

VIM International Vocabulary of Metrology — Basic and general concepts

and associated terms

WCRP World Climate Research Project

WGCV CEOS Working Group on Calibration and Validation

WMO World Meteorological Organization

WOUDC World Ozone and Ultraviolet Radiation Data Center