# Ozone-cci+

# Product Validation Plan (PVP)

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Phase 1, Task 1

Deliverable D1.3

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## DOCUMENT CHANGE RECORD

| Issue | Revision | Date | Modified items | Observations |
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| 1 | 0 | 03/01/2012 | First version | |
| 2 | 0 | 20/01/2020 | Completely revised version to align with CCI+ objectives and with state-of-the-art developments | |
| 2 | 1 | 06/12/2020 | Updated applicable documents (Section 2) and references to the updated URD (Section 3). This version is aligned with URD v3.1. | |
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# Table of Contents

# 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 ESA's Ozone_cci+ project, namely, the vertical column of atmospheric ozone based on nadir satellite measurements, and its vertical distribution based on nadir and on limb/occultation satellite measurements. This plan is a significant update of the earlier version developed and applied in the framework of the former Ozone_cci project, now aligned with the objectives of the CCI+ programme.

## *1.2 Document overview*

This Ozone_cci+ Product Validation Plan is organised as follows:

- Chapter 1 contains this introduction describing the scope of the document.
- Chapter 2 lists applicable and reference documents.
- 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.
- Chapter 5 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.
- Chapter 6 checks the compliance of this document with requirements expressed in the Statement Of Work of the CCI programme and its ozone related annexes.
- Chapter 7 defines the recommended terminology, abbreviations and acronyms.

# 2 Applicable and reference documents

## 2.1 Applicable documents

[RD1] CCI+ SoW: Climate Change Initiative Extension (CCI+) Phase 1 – New R&D on CCI ECVs – Statement of Work, ESA-CCI-EOPS-PRGM-SOW-18-0118, 31/05/2018 + Annex B: Ozone ECV (Ozone_cci).

[RD2] CCI+ Baseline Proposal: CCI+ Phase 1 – New R&D on CCI ECVs : Ozone ECV – Baseline Proposal – Volume I: Technical Proposal, 86 pp., 14/09/2018.

[RD3] CCI+ Baseline Proposal: CCI+ Phase 1 – New R&D on CCI ECVs : Ozone ECV – Baseline Proposal – Volume II: Management and Administrative Proposal, 86 pp., 14/09/2018.

## 2.2 Reference documents

### 2.2.1 Requirement documents

[RD4] CMUG: Requirement Baseline Document, Deliverable 1.1, Climate Modelling User Group, version 0.6, April 2015.

[RD5] DARD: Ozone CCI Data Access Requirement Document, version 2.1, Ozone_cci_DARD_2.1, 25/05/2016.

[RD6] WMO/GCOS: Public Consultation on the ECV Requirements, https://gcos.wmo.int/en/ecv-review-2020 (last access, 30 November 2020)

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[RD8] URD: Ozone CCI User Requirement Document, Version 3.1, Ozone_cci_URD_3.1, 01/09/2020.

[RD9] WMO: OSCAR (Observing Systems Capability Analysis and Review Tool, https://www.wmo-sat.info/oscar/observingrequirements (last access, 30 November 2020)

### 2.2.2 Standards and framework documents

[RD10] CDRH: Center for Devices and Radiological Health (CDRH), General Principles of Software Validation; Final Guidance for Industry and FDA Staff, CBER CDRH/OC #938, 11/01/2002. Publicly available via http://www.fda.gov/MedicalDevices/DeviceRegulationandGuidance

[RD11] CEOS: Committee on Earth Observation Satellites (CEOS): Terms and Definitions and other documents and resources, publicly available on http://calvalportal.ceos.org

[RD12] GUM: 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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[RD16] VIM: 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

[RD17] WMO Quality Management Framework (QMF), home page at https://public.wmo.int/en/our-mandate/how-we-do-it/quality-management-framework

[RD18] 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. 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)

[RD19] ISO Quality Management Principles available at https://asq.org/quality-resources/iso-9000 and https://asq.org/quality-resources/iso-14000

[RD20] NetCDF Climate and Forecast Metadata Convention, http://cfconventions.org

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[RD22] World Meteorological Organization, WMO Global Atmosphere Watch (GAW) Implementation Plan: 2016-2023, GAW Report No. 228, https://library.wmo.int/doc_num.php?explnum_id=3395.

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# 3 User requirements

## *3.1 General requirements*

ECVs produced within the Ozone_cci+ project consist of (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) [RD8] defines climate user requirements, based on the ozone requirements of the Global Climate Observing System [RD6], the CCI Climate Modelling User Group (CMUG) [RD4], the Integrated Global Atmospheric Chemistry Observation theme (IGACO) of the Integrated Global Observing Strategy (IGOS) [RD7], and the WMO rolling requirements [RD9]. 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 (δTOC) such that TOC ± δTOC represents at least a 95% confidence interval. This δTOC value contains a systematic term and a random term, corresponding to classical bias and precision (2σ 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 (e.g., ±500 m for limb retrievals), the other representing a volume mixing ratio range (requirements between 8% and 16%), and both representing a ±95% 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.

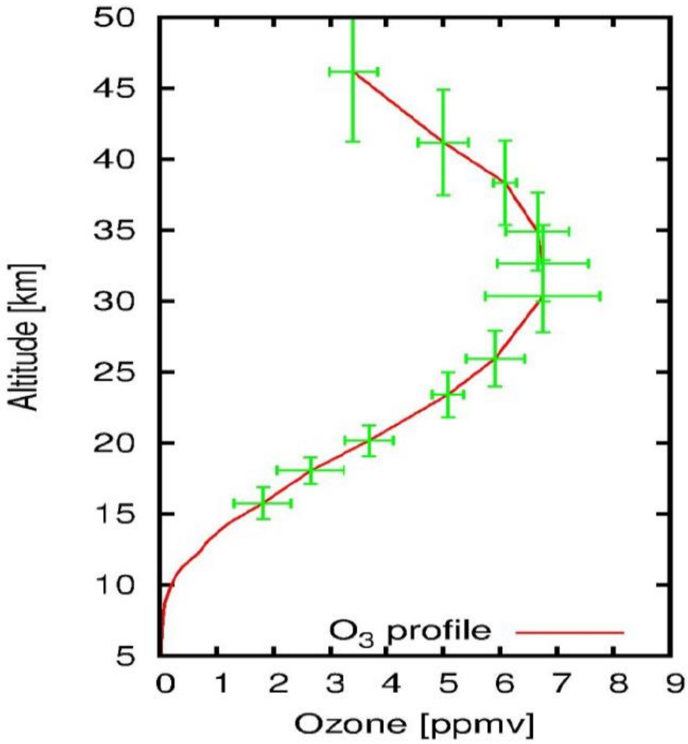


**Figure 1** *Illustration of an ozone profile and the reporting of errors (from URD version 3.1, 2020).*

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 daily to weekly 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 3% for total ozone data and up to 8-16% for vertical profile ozone data.
- Geographical domain: global, regional, latitude-height monthly mean cross-sections.
- Horizontal resolution requirements: from 20 km to 400 km depending on the ECV.
- Vertical range and sensitivity: requirements reflect the vertical structure of ozone changes, namely total ozone column (TOC), and ozone in the troposphere (surface to tropopause), in the upper troposphere / lower stratosphere (UTLS, 5-30 km), in the lower stratosphere (LS, between tropopause and 30 km) and in the upper atmosphere (UA, 30-60 km). The tropopause is defined by the (pressure) altitude that satisfies the temperature lapse rate criterion by WMO (< 2K/km) or by the (pressure) altitude above which the ozone volume mixing ratio continues to exceed 150 ppbv.
- 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 long-term data sets for ozone-climate interactions (Level-3 and Level-4).
- 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.
- Requirements for ancillary data: e.g., 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 3.1 of the URD (Tables 5 to 10), against which the 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).

The URD tabulates quantitative requirements for the *accuracy* of a data product, even though international standards such as the BIPM/ISO VIM [RD16] and GUM [RD12]) specify that accuracy is not considered a quantity and that is not given a numerical value (see Table 10). Furthermore, the URD specifies that required precision is always the same as for the tabulated “accuracies” under the assumption that the important biases in the products will be fully characterized. The PVP therefore interprets the requirements in the URD as requirements on *total uncertainty*, being the squared sum of systematic error estimate and random uncertainty. All requirements represent 95% confidence intervals, equivalent to two times the standard deviation of a Gaussian distribution.

## 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 '–', the first number is the future target. Total uncertainty requirements represent 95% confidence (Adapted from URD version 3.1, 2020).*

| Quantity | Driving Research topic | Geographical Zone | | |
|---|---|---|---|---|
| | | Tropics | Mid-latitudes | Polar latitudes |
| Global horizontal resolution | Evolution of the ozone layer (radiative forcing); Seasonal cycle and interannual variability; Short-term variability* | 20 – 100 km | 20 – 50/100 km | 20 – 50/100 km |
| Observation frequency | Evolution of the ozone layer (radiative forcing); Seasonal cycle and interannual variability; short-term variability* | Daily to weekly | Daily to weekly | Daily to weekly |
| 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 |

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

**Table 2.** *Data format and metadata requirements for total ozone. (From URD version 3.1, 2020)*

| Data feature | Requirement |
|---|---|
| Data format | netCDF [RD20] |
| Data conventions | CF |
| Data units | Total column (in DU; number of molecules per area or equivalent) |
| Error | Total area |
| Error characteristics (optional) | Total uncertainty and its subdivision per pixel into:<br>- contribution measurement noise;<br>- contribution of a priori uncertainties;<br>- 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<br>2: contaminated data<br>3: missing value |
| Visualisation | Basic browsable archive visualisation (daily global maps; local/latitudinal time series of monthly means); this requires that the data are stored in geo-referenced arrays, instead of the per pixel/per scan type. |

## *3.3 Ozone profile data product from nadir-viewing instruments*

**Table 3.** *Product requirements for nadir-based ozone profiles. The required coverage is global. Achievable and future target requirements are given, separated by a '–', the first number is the future target. Total uncertainty requirements represent 95% confidence (From URD version 3.1, 2020).*

| **Quantity** | **Driving Research topic** | **Height range** | | |
|---|---|---|---|---|
| | | **Troposphere** (surface – tropopause**) | **UTLS** (5-30km) | **Middle Atmosphere** (30-60 km) |
| Horizontal resolution | Regional differences in evolution of the ozone layer and tropospheric ozone burden (radiative forcing); Seasonal cycle and interannual variability; Short-term variability* | 20 – 200 km | 20 – 200 km | 200 – 400 km |
| Vertical resolution | Height dependence of evolution of the ozone layer and the tropospheric ozone burden (radiative forcing); Seasonal cycle and interannual variability; Short-term variability* | 6 km – tropospheric column | 6 km – partial column | 6 km – partial column |
| Observation frequency | Evolution of the ozone layer and the tropospheric ozone burden (radiative forcing); Seasonal cycle and interannual variability; Short-term variability* | Daily to weekly | Daily to weekly | Daily to weekly |
| Time period | Evolution of the ozone layer and tropospheric ozone burden (radiative forcing) | (1980-2010) – (1996-2010) | (1980-2010) – (1996-2010) | (1980-2010) – (1996-2010) |
| Total uncertainty | Evolution of the ozone layer and tropospheric ozone burden (radiative forcing) | 8 % | 8 % | 8 % |
| Total uncertainty | Seasonal cycle and interannual variability; Short-term variability* | 16 % | 16 % (<20 km) 8% (>20 km) | 8 % |
| Stability | Evolution of the ozone layer and tropospheric ozone burden (radiative forcing); trends | 1 – 3 % / decade | 1 – 3 % / decade | 1 – 3 % / decade |

* Short-term variability includes : exchange of air masses, streamers, regime studies.
** Tropopause is defined by the (pressure) altitude that satisfies the temperature lapse rate criterion by WMO (< 2K/km) or by the (pressure) altitude above which the ozone volume mixing ratio continues to exceed 150 ppbv.

**Table 4.** *Data format and metadata requirements for nadir-based ozone profiles. (From URD version 3.1, 2020)*

| **Data feature** | **Requirement** |
|---|---|
| Data format | netCDF [RD20] |
| Data conventions | CF |
| Data units | Ozone mixing ratio (optional: also in partial ozone column and/or with co-located temperature profile) |
| Error characteristics | Total uncertainty and its subdivision per pixel and per layer into:<br>- contribution of the measurement noise;<br>- contribution of the smoothing error<br>- contribution of the 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) |

## 3.4 Ozone profile data product from limb-viewing instruments

**Table 5.** *Product requirements for limb-based ozone profiles. The required coverage is global. Achievable and future target requirements are given, separated by a '–'. The first number is the future target. Total uncertainty requirements represent 95% confidence (Adapted from URD version 3.1, 2020).*

| **Quantity** | **Driving Research topic** | **Height Range** | |
|---|---|---|---|
| | | **Lower Stratosphere** (tropopause – 30 km) | **Middle Atmosphere** (30-60 km) |
| Horizontal resolution | Regional differences in the evolution of the ozone layer (radiative forcing); Seasonal cycle and interannual variability; Short-term variability* | 100 – 200 km | 200 – 400 km |
| Vertical resolution | Height dependence of evolution of the ozone layer (radiative forcing); Seasonal cycle and interannual variability; Short-term variability* | 1 – 2 km | 2 – 4 km |
| Observation frequency | Seasonal cycle and interannual variability; short-term variability* | Daily to weekly | Daily to weekly |
| Time period | Evolution of the ozone layer (radiative forcing) | (1980-2010) – (2003-2010) | (1980-2010) – (2003-2010) |
| Total uncertainty in height attribution | Evolution of the ozone layer (radiative forcing), Seasonal cycle and interannual variability; Short-term variability* | ±500 m | ±500 m |
| Total uncertainty on mixing ratio | Evolution of the ozone layer (radiative forcing) | 8% | 8% |
| Total uncertainty on mixing ratio | Seasonal cycle and interannual variability; Short-term variability* | 16 % (<20 km)<br>8% (>20 km) | 8 % |
| Stability | Evolution of the ozone layer (radiative forcing); trends | 1 – 3 % / decade | 1 – 3 % / decade |

* Short-term variability includes : exchange of air masses, streamers, regime studies.
** Tropopause is defined by the (pressure) altitude that satisfies the temperature lapse rate criterion by WMO (< 2K/km) or by the (pressure) altitude above which the ozone volume mixing ratio continues to exceed 150 ppbv.

**Table 6.** *Data format and metadata requirements for limb-based ozone profile requirements. (URD version 3.1, 2020)*

| **Data feature** | **Requirement** |
|---|---|
| Data format | netCDF [RD20] |
| Data conventions | CF |
| Data units | Ozone mixing ratio (optional: also in partial ozone column and/or with co-located temperature profile) |
| Error characteristics | Total uncertainty and its subdivision per profile per layer into:<br>- contribution of the measurement noise;<br>- contribution of the horizontal smoothing error<br>- contribution of the pointing accuracy<br>- contribution of the 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) |

# 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 continues 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.

## *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) [RD18] establishes general principles of the data quality strategy for the Global Earth Observation System of Systems (GEOSS). The core requirement of QA4EO is that all data and derived products shall have associated with them a documented and fully traceable quality indicator (QI). This quality indicator shall provide sufficient information to allow all users to readily evaluate the “fitness for purpose” of the data or derived product. The 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 the URD. Uncertainty estimates can include, but are not restricted to, estimates of the bias and dispersion 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 [RD16].

### 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 [RD87]. In the context of CCI, quality must be evaluated also through critical analysis of the suitability of the data products for the targeted applications, i.e. through the validation of the actual usability of the datasets.

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.

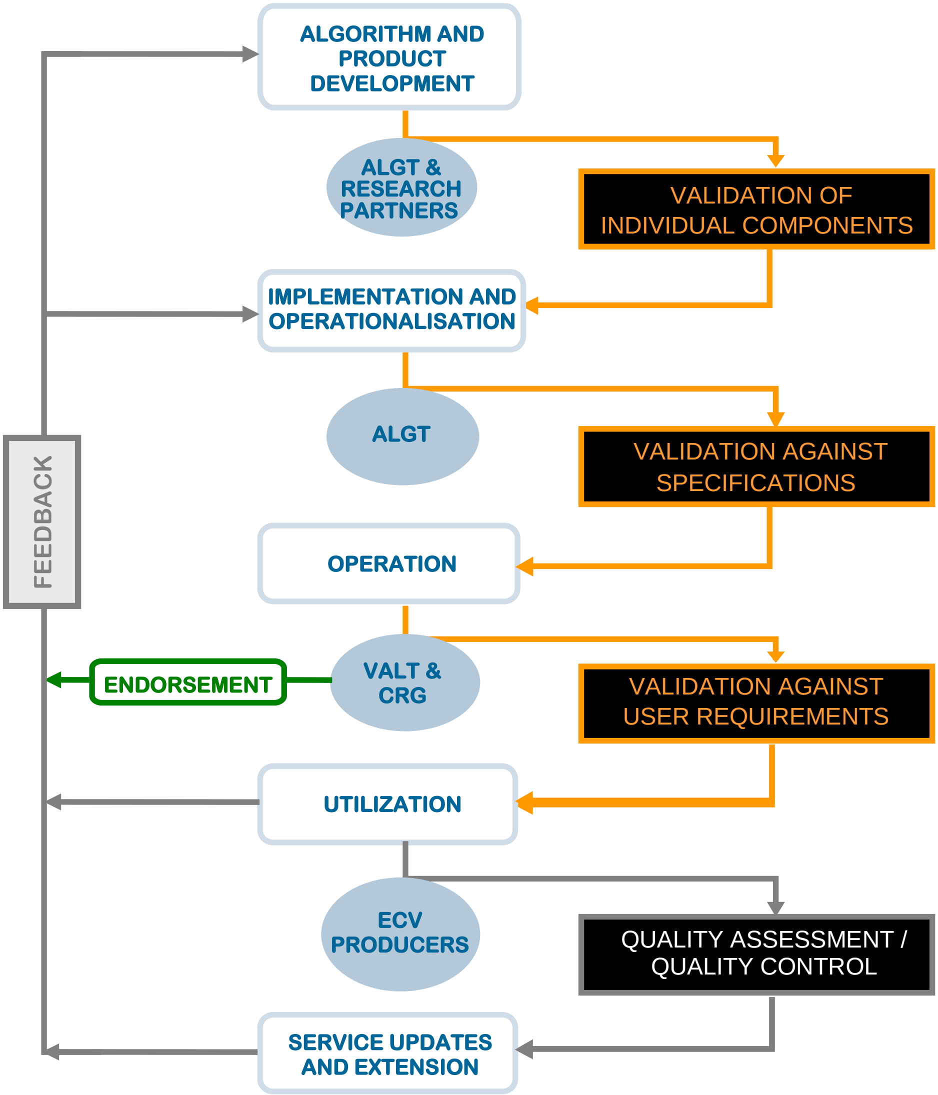


**Figure 2** *Validation tasks, quality control mechanisms and feedback loops over the life cycle of an ozone ECV production line.*

From top to bottom, the box chart shows the timeline for the evolution of an ECV production chain (centre column blue square boxes) through phases from the build-up through operations to updates and its associated validation steps (right-hand column of orange square boxes). The high level appointment of responsibilities is outlined in the centre column (oval boxes), highlighting the respective role of research partners, of system developers and ECV data producers (ALGT), 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 detail.

### 4.2.4 Confrontation with independent reference data

#### *4.2.4.1Generalities*

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 differences in sampling, 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 our current ability to model/algorithmically depict this understanding and they can suffer from many limitations and uncertainties.

#### *4.2.4.2Reference 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) [RD22]. 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) [RD5]. 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.

#### *4.2.4.3Error budget of a data comparison*

A major objective of quantitative comparisons with reference measurements is to estimate the validity of the theoretical (ex-ante) uncertainties provided with the data product. However, the discrepancy between the satellite data set being validated and the reference data set combines uncertainties associated with each individual system, plus uncertainties associated with 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.

(2) Comparison uncertainties associated with the difference in smoothing of atmospheric variability and structures: e.g., balloon-based in situ measurement at about 150 m resolution by an electrochemical cell, compared with GOME ground pixels of 40 x 320 $km^2$ or TROPOMI ground pixels of 5.5 x 3.5 $km^2$ and a vertical resolution of 3-8 km.

As much 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.) [RD46].

Although essential, the derivation of a complete error budget for each comparison is still a matter of research at the time being [RD39] and it falls partly beyond the scope of the Ozone_cci+ project. Validation teams (VALT) as well as data producers (ALGT) 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 – actual 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.

#### *4.2.4.4Information 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 shapes 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 either not at all or less sensitive due to optically thick clouds or too low signal-to-noise ratios, it is important to understand what information, in the final product, is derived from the climatology and what is really contributed bythe 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 [RD44]. For example, 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.

### 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 researchers 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 the Product Specification Documents (PSD) and the 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 [RD8].

### 4.2.7 Validation against user requirements

User requirements are defined in the URD [RD8], on which summary tables reproduced in Section 3 are based. Products need to be validated against these official user requirements. Assessment of compliance with requirements on observation frequency is straightforward. Compliance with requirements on total uncertainty 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 the information content. Compliance with more specific requirements, e.g., in terms of actual geographical coverage and of point-to-zone representativeness, may require 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 the 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.

## 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:

- 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.
- Statistical estimators of the difference like the bias and the dispersion 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 the 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.
- 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. In particular, 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.
- Decadal stability of the bias 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 dispersion shall be assessed, including annual cycle, interannual variability and shorter term variability of the bias.
- 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

The DARD [RD5] describes the reference measurements to be used for validation studies and/or for cross-comparison studies, with details on their access. The following measurement data sets will be used:

- 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.
- Ground-based ozone column measurements by UV-visible DOAS spectrometers.
- Satellite ozone column data by non-CCI retrieval algorithms for EOS-Aura OMI, Metop GOME-2 series, and Suomi-NPP OMPS-NM.

### 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:

- 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.
- 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.
- Studies shall address ozone in the troposphere, in the UTLS and in the middle atmosphere.
- 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 retrieval altitude, as expressed by the centroid or the peak altitude of the averaging kernels, from the nominal retrieval altitude. Dependences on time, SZA, latitude, … should be identified.
- Statistical estimators of the difference like the bias and the dispersion 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.
- 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. In particular, 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.
- 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 dispersion shall be assessed, including annual cycle, interannual variability and shorter term variability of the bias.
- 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*

The DARD [RD5] describes the reference measurements to be used for validation studies and/or for cross-comparison studies, with details on their access. The following measurement data sets will be used:

- Ground-based ozone profile measurements by balloon-borne ozonesondes.
- Ground-based ozone profile measurements by stratospheric ozone lidars.
- Ground-based ozone profile measurements by ozone microwave radiometers.

### 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:

- 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.
- Studies shall address at least ozone in the lower stratosphere and in the middle atmosphere.
- Statistical estimators of the difference like the bias and the dispersion 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.
- 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. In particular, the dependence of the ECV data quality on measurement and retrieval parameters shall be investigated.
- Decadal stability of the bias 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 dispersion shall be assessed, including annual cycle, interannual variability and shorter term variability of the bias.
- 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*

The DARD [RD5] describes the reference measurements to be used for validation studies and/or for cross-comparison studies, with details on their access. The following measurement data sets will be used:

- Ground-based ozone profile measurements by balloon-borne ozonesondes.
- Ground-based ozone profile measurements by stratospheric ozone lidars.
- Ground-based ozone profile measurements by ozone microwave radiometers.

# 5 Standards

## *5.1 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 widening 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 [RD20] in the Ozone_cci project).

## *5.2 Metadata and additional information*

Important information on ECV data and their quality must be readily accessible. 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:

- Identify and locate the datasets or services they need ("discovery metadata").
- 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).
- Retrieve and read the data (format metadata) or access the products provided.
- Understand and interpret the data and their limitations (scientific metadata).
- Seek further information or help if required (references, links, contact).

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

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

## *5.3 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 .png 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 an 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 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.

## *5.4 Compliance with international standards*

Interoperability is a driving concept of the GEOSS Implementation Plan in general and of the CCI/CCI+ programme 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.

Particular attention must be paid 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. Data themes under Annex III of the IRs 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. The NetCDF formats adopted in Ozone_cci are compliant with INSPIRE IRs.

**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 and smoothing (vertical and horizontal, e.g. using a Gaussian, averaging kernels etc.), domain 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)… |

# 6 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) and specific requirements in Annex B for the Ozone ECV (Ozone_cci) (Table 9).

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

| | REQUIREMENT | COMPLIANCE | REMARKS |
|---|---|---|---|
| **R20** | Each project shall validate their ECV products against independent measurements | Full | |

**Table 9** *Specific requirements in Annex B of the Ozone ECV (Ozone_cci) Statement Of Work* [RD1].

| | REQUIREMENT | COMPLIANCE | REMARKS |
|---|---|---|---|
| **TR23** | The contractor shall update the plan for the validation of contributing satellite data products.<br>In detail this shall include an improvement of uncertainty estimates and the relevance for validation activities. Potentially include OSSE simulations to improve the error budget. | Full | The OSSSMOSE system will be used in an attempt to quantify co-location mismatch errors and/or sampling errors for total column ozone products. |
| **TR24** | The relevance for trend studies with Ozone_cci products shall be assessed. | Full | |
| **TR25** | The contractor shall asses the need for a round-robin exercise for all ozone products including updated and new algorithms. As an outcome of the assessment it will be discussed how the round-robin exercise is to be performed. Specifically the limb/nadir synergy shall be assessed to derive tropospheric ozone data. | Full | The need to perform an eventual robin-robin exercise on OMPS-LP retrieval algorithms will be investigated. |

# 7 Terms and definitions

## *7.1 Terms and definitions*

In Table 10 terms and definitions as recommended by CEOS WGCV and by standards development organisations of international recognition have been transcripted from reference documents [RD10] to [RD18]. 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 10.** *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 |
| bias | (1) systematic error of indication of a measuring system<br>(2) estimate of a systematic measurement error<br>(3) estimate of a systematic forecast error | VIM<br>VIM<br>GAS |
| calibration | (1) the process of quantitatively defining the system responses to known, controlled signal inputs<br>(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 | CEOS<br>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 |
| detection limit | measured quantity value, obtained by a given measurement procedure, for which the probability of falsely claiming the absence of a component, given a probability α of falsely claiming its presence | VIM |
| error | (1) measured quantity value minus a reference quantity value<br>(2) difference of quantity value obtained by measurement and true value of the measurand<br>(3) difference of forecast value and a, estimate of the true value | VIM<br>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 |
| influence quantity | 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 |

| TERM | DEFINITION | SOURCE |
|---|---|---|
| in situ measurement | (1) a direct measurement of the measurand in its original place<br>(2) any sub-orbital measurement of the measurand | GEOSS |
| 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<br>(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 pre-determined 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<br>(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 |

| TERM | DEFINITION | SOURCE |
|---|---|---|
| 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<br>(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)<br>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<br>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 |
| validation | (1) the process of assessing, by independent means, the quality of the data products derived from the system outputs<br>(2) verification where the specified requirements are adequate for an intended use<br>(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.<br>(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 | CEOS<br>VIM<br>NIST<br>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.<br>(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<br>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 |

## *7.2 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 |
| ALGT | Algorithm development Team |
| AMF | Air Mass Factor, or optical enhancement factor |
| ATBD | Algorithm Theoretical Basis Document |
| AUTH | Aristotle University of Thessaloniki |
| BIPM | Bureau International des Poids et Mesures |
| BIRA-IASB | Belgian Institute for Space Aeronomy |
| CCI | ESA's Climate Change Initiative programme |
| CDRH | Center for Devices and Radiological Health |
| CEOS | Committee on Earth Observation Satellites |
| 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 |
| DLR | German Aerospace Centre |
| DOAS | Differential Absorption Optical Spectroscopy |
| DU | Dobson Unit – unit of vertical column density (2.69 $10^{16}$ molec.$cm^{-2}$) |
| EC | European Commission |
| ECSS | European Corporation for Space Standardization |
| Envisat | ESA's Environmental Satellite, launched March 1, 2002 |
| EO | Earth Observation |
| ERS-2 | ESA's Earth Remote Sensing satellite 2, launched April 21, 1995 |
| ESA | European Space Agency |
| ESRIN | European Space Research Institute |
| EUMETSAT | European Organisation for the Exploitation of Meteorological Satellites |
| FMI | Finnish Meteorological Institute |
| 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 |
| 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 |
| I/O | Input/Output |
| IR | INSPIRE Implementation Rule |
| ISO | International Organization for Standardization |
| JCGM | Joint Committee for Guides in Metrology |
| KNMI | Royal Dutch Meteorological Institute |
| Lidar | Light detection and ranging |
| MetOp | EUMETSAT's Meteorological Operational satellite |
| MIPAS | Michelson Interferometer for Passive Atmospheric Sounding |
| MLS | Microwave Limb Sounder |
| MPC | Mission Performance Centre |
| Multi-TASTE | Technical ASsistance To the multi-mission validation of Envisat and Third Party Missions using spectrometers, radiometers and sondes |
| NDACC | Network for the Detection of Atmospheric Composition Change |
| NDSC | Network for the Detection of Stratospheric Change (now NDACC) |
| NOAA | National Oceanic and Atmospheric Administration |
| NRT | Near-real time |
| $O_3$ | ozone |
| OMI | Ozone Monitoring Instrument |
| OPERA | Ozone Profile Retrieval Algorithm |
| PROMOTE | Protocol Monitoring for the GMES Service Element - Atmosphere |
| PSD | Product Specification Document |
| PVP | Product Validation Plan |
| QA4EO | Quality Assurance framework for Earth Observation |
| RAL | Rutherford Appleton Laboratory |
| SAGE | Stratospheric Aerosol and Gas Experiment |
| SBUV | Solar Backscatter Ultraviolet |
| SCIAMACHY | SCanning Imaging Absorption spectroMeter for Atmospheric CHartographY |
| SHADOZ | Southern Hemisphere ADditional Ozonesondes |
| SZA | Solar Zenith Angle |
| TOC | Total Ozone Column |
| TOMS | Total Ozone Mapping Spectrometer |
| 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 |
| 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 |