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DOSSIER: Common

TASK: 2



Atmospheric Monitoring Services

Stage 2 of the Earthwatch GMES Services Element

PROMOTE 2

Atmospheric Services **Validation Protocol**

C5
Version 3
Issue 1




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Atmospheric Services
Validation Protocol

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EXECUTIVE SUMMARY

The second stage of PROtocol MOonitoring for the GMES Service Element (GSE), PROMOTE 2, aims at scaling-up consolidated GMES services for atmospheric monitoring. All services must provide documentary evidence that they fulfil quality standards as well as their own specifications, and that they comply with user requirements. Moreover, sustainable efforts must be envisaged and undertaken to keep service quality at a constant level, and to ensure long term update, availability and traceability of quality information. Appropriate means must be applied during implementation, during operation, and during future updates of the services in order to achieve this quality assurance.

The present C5 *Atmospheric Service Validation Protocol* outlines the top-level definition of the approach for validating all constituents of the PROMOTE-2 S5 *Service Portfolio Specifications*. It establishes validation principles that are universally applicable to all products and services. The present, final version builds on general quality assurance frameworks established by high level bodies and standardisation agencies (e.g., ISO/IEC and QA4EO), on more detailed descriptions suitable for each data product and service (e.g., validation methodologies, plans and reports), and on the experience gained and documents generated during the three annual cycles of PROMOTE 2.


The present protocol is formally agreed by all members of the service supply partnership, including research partners, operational providers, and system developers. It is also endorsed by the mandated representatives of the PROMOTE 2 end-user organisations. This includes, as an absolute minimum, the leaders of the User Executive Board that speaks on behalf of the User Federation. The latter is composed of all users that signed a Service Level Agreement (SLA) within PROMOTE.

This document addresses:

- General rules to ensure unbiased, independent and traceable validation
- Definition of the tasks of the research partners, system developers, service providers and core users regarding the various aspects of the services and data products validation
- Definition of different validation levels and top-level validation criteria, review process and decisions sequence
- Requirements for reference data sources and methods
- Approach for validating new products, upgrades, long-term quality assurance, endorsement by key external user-bodies, validation of services (as opposed to the validation of products only)
- Requirements for appropriate and sustainable validation documentation
- Document availability, access and distribution rules
- Maintenance of validation standards, reports and data sets.

The validation of each service during its build-up and during its successive updates, is fulfilled by a combination of complementary measures, including the end-to-end validation of individual components of a service chain, the validation of data products and services against specifications, and the validation of data products and services against user requirements.

The material in this document has been subject to technical and policy review by ESA, the PROMOTE Core Management Team and the PROMOTE Service Leaders, and approved for publication with open diffusion. The views expressed by the authors, however, are their own, and do not necessarily reflect those of ESA and of all contributors.

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DOCUMENT CHANGE RECORD

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1	0.0	16.08.2006	Document created
1	0.1	31.10.2006	Draft reported to PROMOTE 2 PM1 (Vienna, 02-03.11.2006)
1	A	30.11.2006	First public issue delivered to ESA
2	0.1	29.06.2007	INSPIRE; material from CEOS WGCV 27 (Teddington, 12-15.06.2007)
2	0.2	01.03.2008	ISO; CDHR; material from CEOS WGCV 28 (Sanya, 26-29.02.2008)
2	0.3	13.04.2008	Updates based on feedback from PROMOTE validation cycle 1
2	0.4	03.06.2008	NIST; material from GEO-CEOS workshops at GEO-Sec and NIST
2	0.5	07.07.2008	VIM; material from INSPIRE conference (Maribor, 22-26.06.2008)
2	0.6	08.10.2008	Draft reported to PROMOTE 2 AM2 (Brussels, 08-09.10.2008)
3	0.1	10.12.2008	Updates based on feedback from PROMOTE validation cycle 2
3	0.2	21.04.2009	INSPIRE IRs; GIGAS workshop (Brussels, 28/29.01.2009)
3	0.3	07.07.2009	QA4EO; material from CEOS WGCV 30 (Ilhabela, 26-29.05.2009)
3	0.4	12.10.2009	Provisional issue for review and endorsement (reviewers listed on Page 2)
3	1.0	14.10.2009	Final version


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1. INTRODUCTION

1.1 Purpose of this document

PROMOTE Atmospheric Services

The *GMES Service Element for Atmosphere*, PROMOTE 2, delivers policy-relevant services on a variety of atmospheric issues addressing the thematic domains of ozone, ultraviolet radiation, air quality, climate change, and aviation hazards due to volcanism. PROMOTE 2 services integrate observations by ground-based networks and by satellites with a hierarchy of models. They cover spatial scales from the ozone hole – at continental scale – to polluted streets and temporal scales from climate and ozone trends across decades to hourly information on ultraviolet radiation levels on Mediterranean beaches. Services deliver either quantitative data directly to public authorities and other institutions, or easily understandable information to European citizens via local environment and health agencies.

User Needs


A major challenge in the life cycle of a user-oriented service is to provide sound description and quantification of the data products and their uncertainties that users need to take into account. Among users targeted by PROMOTE 2, over sixty core user organisations are involved actively in the project via a formal Service Level Agreement (SLA), in which user needs are outlined.

Service Validation Protocol

The present *Service Validation Protocol* (PROMOTE-2 document C5) outlines the top-level definition of the approach for validating all constituents of the *Service Portfolio Specifications* (S5). It establishes validation principles that are universally applicable to all products and services, plus specific principles more dedicated to families of services. Established by an independent Quality Assessment and Validation Office on the basis of documentation, accepted practices and international standards collected from authorised sources, the *Service Validation Protocol* is endorsed by the service networks and by their users.

Restrictions

The present *Service Validation Protocol* does not claim to address safety concerns, if any, associated with the use of the PROMOTE data and services. It is the responsibility of the service provider to document appropriately the scope and validity of the data delivered. And it is the responsibility of the user to establish appropriate data interpretation, safety and health practices, and to determine the applicability of reported limitations prior to use.

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1.2 Document overview

This document is organised as follows:

Chapter 1 contains this introduction, with a list of applicable and reference documents.

Chapter 2 summarises the generic principles of the validation protocol and explains the specifics with regard to validation of the five thematic lines in the Service Portfolio.

Chapter 3 addresses the responsibilities for the different aspects and tasks of validation.

Chapter 4 details the general principles of quality control rules.

Chapter 5 addresses validation and quality control standards: sustainable archiving and traceability quality of the validation process and of validation results, quality control metadata and criteria, quality assurance breakpoints, and documentation.

Abbreviations and Acronyms, and Terms and Definitions, are listed in the Annexes.

1.3 Applicable and Reference Documents


1.3.1 Applicable Documents

- [AD1] ESA's Statement Of Work "Scaling-up Consolidated GMES Services for Humanitarian Aid and Atmospheric Monitoring", EOEP-GSE-EOAD-SW-05-0001, Issue 2.1, Nov 18, 2005.
- [AD2] The Prime Contractor's proposal, ref. 3400720, dated March 8, 2006, as amended by Revision 1, ref. 3 400 720 Rev. 1, dated June 19, 2006, and the minutes of the kick-off meeting held on July 18, 2006, at DLR.
- [AD3] U1 Core User Needs and User Standard Dossier
- [AD4] C7 (draft + finalised) Service Level Agreements for each of end user organisation
- [AD5] D2 Service Network Configuration Master Document; S3 Service Prospectus
- [AD6] S5 Service Portfolio Specifications
- [AD7] S6 Service Operations Report
- [AD8] U7 Service Utility Reports

1.3.2 Reference Documents

1.3.2.1 PROMOTE documents

- [RD1] U1 Core User Needs and User Standard Dossier
- [RD2] C7 (draft + finalised) Service Level Agreements for each of end user organisation
- [RD3] D2 Service Network Configuration Master Document; S3 Service Prospectus
- [RD4] S5 Service Portfolio Specifications
- [RD5] S6 Service Operations Report
- [RD6] U7 Service Utility Reports


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1.3.2.2 Service specifications (ATBDs, PSDs...)

Algorithm Theoretical Basis Document (ATBD), Product Specification Document (PSD) etc., as referred to on <http://www.gse-promote.org> on the home page of every PROMOTE atmospheric service.

1.3.2.3 Framework documents, standards, terms and definitions


- [RD7] 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/>
- [RD8] Committee on Earth Observation Satellites (CEOS): Terms and Definitions and other documents and resources publicly available on <http://calvalportal.ceos.org>
- [RD9] INSPIRE: Web portal of the Infrastructure for Spatial Information in the European Community (INSPIRE), <http://inspire.jrc.ec.europa.eu>, and INSPIRE Geoportal, <http://www.inspire-geoportal.eu>. The INSPIRE framework includes common Implementing Rules (IR) adopted in the areas of Metadata, Data Specifications, Network Services, Data and Service Sharing, and Monitoring and Reporting.
- [RD10] ISO Quality Management Principles available at <http://www.iso.org/iso/iso9000-14000/understand/qmp.html>
- [RD11] Larssen, S., R. Sluyter, and C. Helmis, Criteria for EUROAIRNET – The EEA Air Quality Monitoring and Information Network, 1999.
- [RD12] Nappo, C.J., Caneill J.Y., Furman R.W., Gifford F.A., Kaimal J.C., Kramer M.L., Lockhart T.J., Pendergast M.M, Pielke R.A., Randerson D., Shreffler J.H., and Wyngaard J.C., The Workshop on the Representativeness of Meteorological Observations, June 1981, Boulder, CO, Bull. Am. Meteorol. Soc. 63, 761-764, 1982.
- [RD13] NIST: Prokhorov, A. V., R. U. Datla, V. P. Zakharenkov, V. Privalsky, T. W. Humpherys, and V. I. Sapritsky, Spaceborne Optoelectronic Sensors and their Radiometric Calibration. Terms and Definitions. Part 1. Calibration Techniques, Ed. by A. C. Parr and L. K. Issaev, NIST Technical Note NISTIR 7203, March 2005.
- [RD14] 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)
- [RD15] 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>
- [RD16] WMO Quality Management Framework (QMF), home page at <http://www.wmo.int/pages/prog/www/QMF-Web/home.html>

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1.3.2.4 Validation methods and validation results

Common, acceptable practices in validation and validation results can be found in the following reference documents generated by service networks, by supporting projects with a clear link to PROMOTE-like activities, and by external projects without direct link to PROMOTE.


- [RD17] ACCENT, Atmospheric Composition Change, the European Network of Excellence, EU FP6 project, home web page at <http://www.accent-network.org/>
- [RD18] ACCENT TROPOSAT-2 (AT-2), Atmospheric Composition Change, the European Network of Excellence – Remote Sensing of Atmospheric Constituents from Space, <http://troposat.iup.uni-heidelberg.de/AT2/index.html> See AT-2 Book, issued in 2009, including Chapter 7 dedicated to the validation of tropospheric observations from satellites.
- [RD19] AERO-SAM, Boundary layer AEROSol characterization from Space by advanced data Assimilation into a tropospheric chemistry transport Model, DFG-Project (October 2004 – November 2007)
- [RD20] AGAGE, Advanced Global Atmospheric Gases Experiment network, funded partly by NASA in the US and partly by the governments of Australia, United Kingdom and Japan, home web page at <http://agage.eas.gatech.edu/>
- [RD21] ASSET, Assimilation of Envisat data, EU FP5 project, home web page at <http://darc.nerc.ac.uk/asset/>
- [RD22] ASTHMA, Advanced system of teledetection for healthcare. Management of asthma, service home web page at <http://www.enviport.com/cgi-bin/exe.pl?asthma&en&asthma&0>
- [RD23] ASTM International – Standards Worldwide (ASTM), home page at <http://www.astm.org>
- [RD24] Atmospheric Water Vapour Literature Database on <http://www.watervapour.org>
- [RD25] Axe Santé-Environnement, Etudes et Recherche en Pathologies de l'Université de Rouen (ERPUR), service home web page at http://www.univ-rouen.fr/79479574/0/fiche_UFM_pagelibre/
- [RD26] BASCOE, Belgian Assimilation System of Chemical Observations from ENVISAT, service home web page at <http://bascoe.oma.be/>
- [RD27] BILRUSIA, Aerosol modelling, Belgian national funded project
- [RD28] CHEOPS-GOME, Climatology of Height-resolved Earth Ozone and Profiling Systems for GOME, ESA project, web page at <http://nnorsy.zsw-bw.de/GOME.html>
- [RD29] COPS, model assimilation of EO & ground-based data (ESA)
- [RD30] COST726, Long term changes and climatology of UV radiation over Europe, EU Cost Actions, home web page at <http://i115srv.vu-wien.ac.at/uv/COST726/Cost726.htm>
- [RD31] COST728, Meso-scale meteorological modelling for air pollution and dispersion application, EU Cost Actions, home web page at <http://www.cost728.org/>

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- [RD32] COST Action ES0604, Water Vapour in the Climate System (WaVaCS), COST web page at http://cost.esf.org/index.php?id=205&action_number=ES0604, WaVaCS web page at <http://www.isac.cnr.it/wavacs/>
- [RD33] CREATE/DAEDALUS, Construction, use and delivery of a European aerosol database/ Delivery of AErosol proDUcts for Assimilation and environmental Use, EU FP5 project, home web page at <http://loacli.univ-lille1.fr/Daedalus/Daedalus/index.html>
- [RD34] DOMINO, Derivation of Ozone Monitoring Instrument tropospheric NO₂ in near-real time, 2004-2005, funded by the Dutch NIVR, home web page at <http://www.knmi.nl/~eskes/projects/domino.html>
- [RD35] ENVIRONMENT & HEALTH, long-term high resolution AQ simulation, Belgian national funded project
- [RD36] EVERGREEN, EnVisat for Environmental Regulation of GREENhouse gases, EU FP5 project, home web page at <http://www.knmi.nl/evergreen/>
- [RD37] EXUPERY, SO₂ algorithm development for GOME-2, monitoring volcanic plumes, BMBF-Geotechnologien
- [RD38] GAW, Global Atmosphere Watch, http://www.wmo.ch/web/arep/gaw/gaw_home.html
- [RD39] GEOmon, Global Earth Observation and Monitoring of the Atmosphere, EU FP6 Integrated Project, home web page at <http://www.geomon.eu>
- [RD40] GlobAER, A unified, global aerosol dataset from MERIS, (A)ATSR and SEVIRI, ESA Data User Element programme, home web page at <http://www.globaerosol.info/>
- [RD41] IMACCO, Virtual institute for Inverse Modelling of the Atmospheric Chemical Composition, home web page at <http://www.fz-juelich.de/icg/icg-ii/imacco/>
- [RD42] ISSI Working Group on Atmospheric Water Vapour web page at <http://www.iapmw.unibe.ch/research/projects/issi/>
- [RD43] KOPRA project on integrated modelling of particulate matter in Finland, service home web page at <http://www.ymparisto.fi/default.asp?node=12463&lan=en>
- [RD44] MUSTI, Belgian AQ forecast
- [RD45] NDACC, Network for the Detection of Atmospheric Composition Change, home web page at <http://www.ndacc.org>; formerly the NDSC, Network for the Detection of Stratospheric Change (till 2005); sub-menu “NDACC Publications” contains lists of reference papers addressing and illustrating the comparison of measurements by satellites, FTIR spectrometers, UV-visible spectrometers, UV spectrophotometers, sondes, lidar, microwave radiometers, and UV spectroradiometers.
- [RD46] NDACC Satellite Working Group web site at <http://accsatellites.aeronomie.be>
- [RD47] NDMS, Network for the Detection of Mesopause Change, home web page at <http://wdc.dlr.de/ndmc/pags/ndmc-1-home.html>
- [RD48] NNORSY, Neural Network Ozone Retrieval System, home web page at <http://nnorsy.zsw-bw.de>
- [RD49] NOVAC, Network for Observation of Volcanic and Atmospheric Change, EC-funded project, home page at <http://www.novac-project.eu/>
- [RD50] O3M-SAF, Satellite Application Facility on Ozone and Atmospheric Chemistry Monitoring, home web page at <http://o3msaf.fmi.fi>

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- [RD51] OMIVAL, Validation of OMI surface UV data, Finish national funded project, poster at http://www.biospherical.com/nsf/.%5Cpresentations%5CAGU2005_poster_OMUVB2.pdf
- [RD52] QUITSAT, Air quality assessment through the fusion of EO, ground-based & modeling data, Italian project of ASI Italian Space Agency, http://www.cgspace.it/index.php?option=com_content&task=view&id=345&Itemid
- [RD53] SCOUT-O3, Stratospheric-Climate Links with Emphasis on the Upper Troposphere and Lower Stratosphere, EU FP6 project, home web page at http://www.ozone-sec.ch.cam.ac.uk/scout_o3/
- [RD54] SOGE, System for Observation of Halogenated Greenhouse Gases in Europe, part of the cluster of five EU funded projects for Global Atmospheric Observations (GATO), home web page at <http://www.nilu.no/soge/>
- [RD55] SPARC-CCMVal, Chemistry-Climate Model Validation Activity for SPARC (Stratospheric processes and their role in Climate), home web page at <http://www.pa.op.dlr.de/CCMVal/>
- [RD56] TEMIS, Tropospheric Emission Monitoring Internet Service, ESA/ESRIN DUP-II project, home web page at <http://www.temis.nl/>

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2. VALIDATION PROTOCOL

2.1 Foreword

The different services of PROMOTE 2 share several common characteristics: they address similar families of atmospheric species; they use measurements acquired by similar measurement techniques; they rely on modelling results based on a common understanding of atmospheric chemistry and physics; they produce similar outputs. This calls for the definition and implementation of generalised validation principles. Within a thematic line, general principles can be further adapted to thematic specifics. This chapter starts with the general principles applicable to the whole service portfolio and gets on with the specific characteristics applicable for each of the five thematic lines. As a baseline, generic principles and means for validation shall prevail over specific provisions whenever possible, in order to enable a standardised approach.

2.2 General principles of the validation of atmospheric services

2.2.1 Principles of the validation of a service line

Figure 2-1 presents an overview of the major validation tasks to be applied to the PROMOTE 2 service portfolio. From top to bottom, the box chart shows the timeline for the evolution of service development (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 (circle boxes), highlighting the respective role of research partners, system developers, core users and service providers 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 services, to the formal endorsement by their core users, the latter concluding officially the build-up of a service. The following sections describe the major validation tasks in more details.

2.2.2 Principles of the validation of atmospheric data

The validation of an atmospheric data product (e.g. satellite observations and model estimates of the vertical column amount and vertical distribution of an atmospheric trace gas) can be seen as a science-driven verification process, the aim of which being to ensure that the data produced do respond to predefined quality requirements and information content requirements. Validation generally involves the assessment of the accuracy and of uncertainties of the data, over the spatial and temporal domains of relevance. Uncertainty estimates can include, but are not restricted to, estimates of the bias and precision of the data and of the temporal and spatial domains over which those estimates are valid. It must be noted that international standardization 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 it is not given a numerical quantity value. The quality of data sets must be evaluated through analysis of (1) their agreement with “reference” measurements of the same measurand with documented evidence of quality (metrology like validation), and (2) their suitability for the targeted geophysical applications (validation of actual usability).

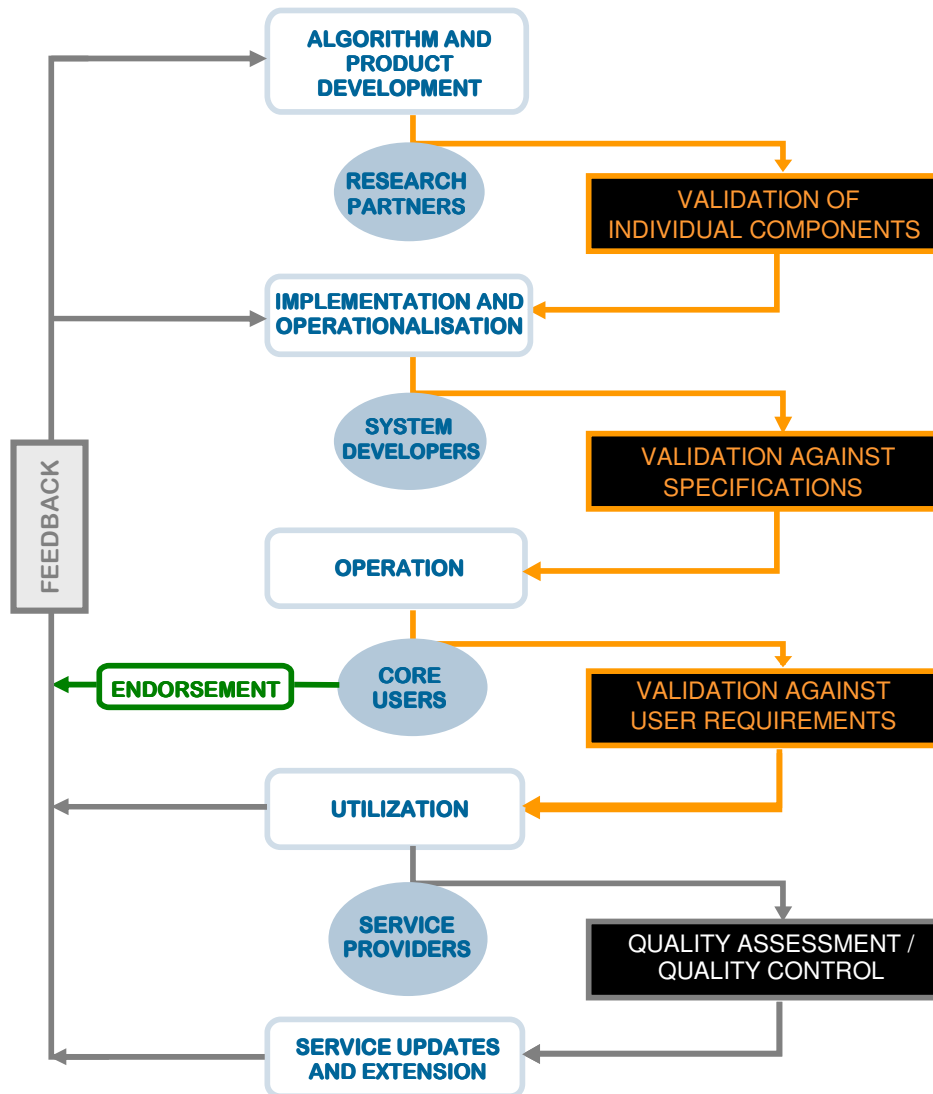



Figure 2-1 – Overview of validation tasks, quality control mechanisms and feedback loops over the life cycle of an atmospheric service.

2.2.2.1 Confrontation with independent reference data

In general the performance of retrieval algorithms and the quality of the resulting data 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 correlative data sets. The quality, traceability and suitability of the latter are essential to allow proper, unbiased and independent validation. Correlative 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. In this case, the principles already stated concerning the selection of correlative data sets apply.

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Where and when correlative observations are available, they constitute the preferred source of validation data, superseding the use of modeling results as validation data. When suitable measurements are not available, validation of data might also involve comparisons with “reference” model data sets (e.g. results from forecast concentrations can be verified by comparison with later analysis of the same quantities). 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 to identify inconsistencies in the data sets under investigation. However models and data assimilation systems must always be used with circumspection in validation as they are based on our own understanding of the atmosphere and they can suffer from many limitations and uncertainties.

It should be pointed out that within the PROMOTE consolidation phase no database with independent validation measurements will be implemented. Therefore PROMOTE needs to completely rely on observations and results provided by existing operational networks and ongoing/planned research projects. Data access/provision agreements and related data policy issues need to be worked out. The participation of several PROMOTE partners in these activities is expected to support this task, but further high-level impetus through ESA and its GSE program is also required, in particular to ensure data provision suitable for sustainable validation activities.

2.2.2.2 Error budget of data comparison

A major objective of quantitative comparisons with correlative data 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 are the result of different families of uncertainty:

- (1) Uncertainties linked to the measurement/modelling (e.g. instrument noise, calibration uncertainties);
- (2) Uncertainties linked to the measurement/modelling parameters (e.g. dependence on the solar zenith angle and the cloud cover, effect of initial and boundary conditions);
- (3) Uncertainties linked to the retrieval (e.g. uncertainties on spectroscopic properties, sensitivity on *a priori* constraints, filtering of incoming observations in a data assimilation scheme);
- (4) Comparison uncertainties associated with the difference in sampling of atmospheric variability and structures (e.g. geographical mismatch, diurnal cycle effects);
- (5) Comparison uncertainties associated with the difference in smoothing of atmospheric variability and structures (e.g. local *in situ* measurement by a sonde at 150m resolution compared with regional modelling on a 1°x1° grid, thus at about 110km resolution in latitude x 70km resolution in longitude).


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Most of comparison uncertainties can 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 (remote sensing or modelling 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 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 beyond the scope of PROMOTE. But validation teams must be 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. Moreover, this awareness should be transmitted to the reader of *C6 Validation Reports* for a proper use of the validation results and, *in fine*, of the atmospheric services. 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.

2.2.2.3 Analysis of information content

Although often ignored, 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 always uses a set of *a priori* constraints, e.g. in the form of an allowed atmospheric variability covariance, an assumed range of atmospheric profile shape, or 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 (1) of comparisons with independent reference data sets, especially during events not considered in the climatology, (2) of the study of deviations of the retrieved product from the *a priori* constraints, and (3) of 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 correlative measurement itself should be known prior to performing a comparison.

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Similar information content studies might be an important aspect in the validation of model runs that have been initialized by a 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 validation of data assimilation results when observations outside of a predetermined range – e.g. during an unexpected Solar Proton Event (SPE) – 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.

2.2.3 Validation of individual service components

Service components are the individual processing blocks by which data products are generated in their interim or final version. For services made of complex chains it is necessary to validate or at least verify the good performance of every component and the accuracy of its output. Validation of only the final data product or the main service product is not sufficient. When produced by a complex retrieval chain, the validation of a single data product is also 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.


The most relevant data products planned for PROMOTE 2 are listed in *S5 Service Portfolio Specifications*. Validation approaches and rules defined in the present document address in priority these products although they can be naturally extended to others, as these will be made available in later stages of the services development. Results of the validation of service components are reported in the *C6 Service Validation Reports*.

2.2.4 Validation against service specifications

Service specifications are outlined in several documents like the *S5 Service Portfolio Specifications*, Algorithm Theoretical Basis Documents (ATBD), and the Product Specification Documents (PSD). A thorough verification of every product specification is out of scope of the present project. The focus will be on service specifications having clear links with user requirements expressed officially through *Service Level Agreements* (SLA) or recognised from the known use of the data products.

2.2.5 Validation against user requirements

User requirements are defined among others through *Service Level Agreements*, which have been endorsed both by registered users and by the service providers. Products need to be validated against these official user requirements. In addition to quality checks on the part of the provider and on the basis of known user requirements, customer feedbacks provide valuable input for the assessment of the service compliance in terms of the accuracy (bias, precision or other estimates) and effective usability of the data product. Such a feedback loop could not be realised in practice during the first stage of PROMOTE. Following recommendations drawn from this first stage and from other parties, a Quality Assessment/Validation Office has been set up in the framework of PROMOTE 2, which supports the different services in establishing a structure linking them to their users in terms of validation.

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2.2.6 Quality control of services in operation


Continuous monitoring of each service component (e.g. retrieval-, 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 provided by each service component. 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 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. At present time, automatic validation procedures still need to be developed/demonstrated.

2.2.7 Validation of service updates

Whenever a major update or upgrade of a service occurs (improved or new algorithm, new sensor, updated photochemical and 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, validation against service specifications, and validation against user requirements. The focus must be logically on the verification of expected product changes. Nevertheless a verification of the entire processing chain might be required. A record of successive updates and corresponding validations should be maintained and made publicly available by the service provider.

2.2.8 Service endorsement by key users

Users shall be involved in the services throughout their entire life cycle (definition, build-up, utilization, upgrades). One particular step of their involvement is after implementation of each sub-service, when an audit will be conducted which should lead to a formal approval of the service by its core users. This may include (according to user requirements) a test operations phase. The consortium does not plan formalized certification following ISO standards for the entire service portfolio or its thematic lines due to the large number of sub-systems and products which are produced on the basis of specific (thematic and regional) user requirements. However, individual sub-systems may choose to undergo a formalised certification, especially when users require this.

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2.3 Specifics of validation of the five thematic lines

2.3.1 Validation of the ozone services

PROMOTE Ozone Services provide **long-term time series** of observations of the ozone vertical column and of the stratospheric ozone profile, and **Near-real-time (NRT) analysis/ short-term forecasts** of the vertical column of atmospheric ozone.


2.3.1.1 Records of ozone column and of stratospheric ozone profile

Long-term data records on the vertical column density of ozone (also called total ozone) and on its stratospheric profile are derived from observations by different satellite missions spanning, all together, over several decades. The stratospheric ozone profile record is produced by assimilation of satellite observations into a system combining meteorological data and chemical transport modelling. Long-term accuracy (stability of bias and precision) of individual satellite data records and of data assimilation results has been established through comparison with numerous ground-based stations contributing to WMO's Global Atmosphere Watch (GAW): the Dobson, Brewer and ozonesonde networks archiving data in the World Ozone and Ultraviolet Data Center (WOUDC), and UVVIS, lidar and other instruments contributing to the Network for the Detection of Atmospheric Composition Change (NDACC). These results are thoroughly documented in the literature and they can serve as a basis for the routine and long-term validation of PROMOTE ozone data records.

In comparison to several other PROMOTE data products, total ozone data derived from satellite observations has now reached a high level of maturity. However present requirements are also highly demanding (long-term stability high enough to detect a 1% trend per decade) and not easy to fulfil and maintain throughout the entire lifetime of the satellite. Therefore an important objective of the validation is the detection of satellite data drifts. Since PROMOTE ozone records integrate data from several satellites, another challenging aspect of the validation is to assess (1) the satellite-to-satellite consistency (bias, noise and stability) as a function of time but also of latitude and of important measurement parameters such as clouds and solar zenith angle, and (2) the impact of relative biases, noise and drifts on the integration of those different data sets. Relative quantification of biases and noise between satellite data sets can be obtained through direct comparisons when data overlap, and also using data assimilation techniques, while absolute quantification of biases, noise and drifts can be obtained through indirect comparisons using ground-based network data as a standard transfer. A special care must be given to effects (e.g. horizontal smoothing errors) of differences in horizontal resolution of the probed air masses, e.g. from 40 x 320 km² for GOME to 17 x 40 km² for OMI.

2.3.1.2 Forecast and NRT analyses of the ozone column

Although not negligible, accuracy requirements on ozone NRT analysis and forecasts are less demanding than those raised by long-term data records. Timeliness of delivery and resolution of the produced ozone fields are evenly important aspects. The reliability of forecasts and NRT analyses requires quick verification (1) against high-quality ground-based measurements at selected GAW/NDACC sites (best maintained Dobson, Brewer and UVVIS stations providing NRT data), and (2) against corresponding assimilated fields, (3) all as a function of time, space and relevant measurement parameters. In-depth validation must be envisaged *a posteriori* to better document and improve the product.

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2.3.2 Validation of the UV services

The **UV-Index** and **Sunburn time** PROMOTE services are directly derived (by multiplying with appropriate factors) from the erythemally weighted (or weighted by another action spectra) and wavelength integrated ultraviolet irradiance data in $W.m^{-2}$. The product **UV-dose** is the ultraviolet irradiance integrated over a given time interval. Algorithms or models providing ultraviolet products use the main ultraviolet-controlling parameters as input. They stem either from satellite observations or forecast models (e.g. total ozone, cloud parameters) as well as from various data bases (e.g. terrain model, climatology of aerosols) and from algorithms based on geographical and astronomical parameters (solar zenith angle, viewing zenith angle). The accuracy of the observations of atmospheric and environmental parameters like total ozone, cloud parameters (optical depth and/or coverage), snow coverage and aerosol optical depth have a direct effect on the accuracy of the derived UV products. As a consequence, the accuracy of UV products, which are provided in accordance to certain service specifications (grid, spatial and temporal resolution, projection etc), is correspondingly determined by the accuracy of the input parameters that are adjusted to these specifications.

2.3.2.1 Verification of radiative transfer models


In the framework of the validation of individual components of a service line, it is a useful task to compare the various radiative transfer models used by the service developers for generating their operational UV algorithms (a core module in each UV service). Usually radiative transfer results have been inter-compared in a predefined range of the main ultraviolet-controlling parameters.

2.3.2.2 UV-irradiance and directly related data products

Since UV-irradiance is the basic quantity from which products as UV-Index and Sunburn-time are derived, a reasonable validation approach is to compare modelled or satellite derived UV-irradiance to precise surface measurements (e.g., spectrally resolved irradiances, UV-A- and UV-B-irradiance, CIE- or other- weighted and integrated irradiances) from well calibrated instruments offering documentary evidence of their traceability to established standards. Ideally, local irradiance measurements are complemented with simultaneous measurements of the main UV controlling parameters. Measurements should be performed at different sites (existing stations) representing different environmental conditions (ozone, clouds, snow, elevation, turbidity) and at different solar local times sampling an adequate range of solar zenith angle. The representativeness of local UV measurements should be considered in view of the service specifications, including those related to spatial resolution. Supporting radiative transfer calculations might be required to interpret and analyse the comparison results.

2.3.2.3 UV doses

The main uncertainties affecting the calculation of daily doses are introduced by the diurnal variation of clouds, total ozone and aerosol optical depth. Therefore correlative surface measurements of UV-irradiance are required at a temporal resolution sufficient to sample meaningfully the diurnal course of these atmospheric parameters. Ideally, ancillary measurements of UV controlling parameters (clouds, albedo, ozone etc.) are performed simultaneously to the UV measurement.

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The representativeness of local UV measurements should be considered in view of the service specifications, including those related to spatial and temporal resolution. In particular, local UV measurements should offer a temporal sampling enabling accuracy assessments of UV-doses at scales from the day to the decade. Supporting radiative transfer calculations might be required to interpret and analyse the comparison results.


2.3.2.4 UV forecasting data products

Timeliness of delivery and resolution of the produced UV forecasts (UV-Indices, sunburn time) are important aspects. The reliability of UV forecasts requires quick verification against continuous surface measurements at adequately selected sites (existing stations representative of scenarios and regions of interest) over a defined period and at a defined sampling rate. Temporal resolution and time periods are defined to enable an assessment of the reliability of forecasted parameters as a function of time and of UV controlling parameters. In-depth validation must be envisaged *a posteriori* to better document and improve the forecast.

2.3.3 Validation of the air quality services

The PROMOTE air quality monitoring and forecast services generate various kinds of data products (trace gas concentrations, aerosol properties and concentrations, indices and pollens). These are derived either from satellites observations (GOME, SCIAMACHY, OMI, ATSR-2, etc), or through assimilation of *in situ* data into atmospheric models (gridded analysis and forecast products). Regional and local air quality model results can be relatively easily validated using surface network measurements usually established by national and regional agencies and harmonised by the European Environmental Agency (EEA). The geophysical validation of satellite measurements of tropospheric species and aerosols is a more challenging task, mainly due to (1) the absence or lack of adequate correlative observations and (2) the large smoothing by satellites and global models of the significant variability (both in time and space) of atmospheric composition, especially in the vicinity of the Earth's surface and of emission sources. The latter difficulty complicates – and often obstruct – the interpretation of comparison results by producing enhanced comparison error bars which can sometimes exceed by one order of magnitude the error bars of the individual measurements.

Available correlative data sets include a combination of *in situ* and remote-sensing techniques from established ground-based, airborne and satellite platforms. In order to ensure meaningful correlative analysis, validation methodologies must account explicitly for (1) the known characteristics (vertical and horizontal resolution/sampling/grid, averaging kernels indicating how the satellite retrieval smoothes actual atmospheric features, temporal sampling etc.) of the satellite observations or of the model, (2) the known characteristics of the correlative measurements, and (3) properties of the atmospheric field (horizontal gradients, vertical structure, upper limit of the planetary boundary layer (PBL), temporal variability...) E.g., local surface observations of the NO₂ concentration in the planetary boundary layer cannot be compared in a straightforward way with tropospheric NO₂ columns derived from GOME scattered-light measurements at its nominal resolution of 40x320 km². In some cases, a combination of several correlative methods and instruments might be required to ensure reliable validation of the satellite data products for a given location. Validation of the individual service components, as well as proper characterisation of both the true information content and the atmospheric environment, are certainly key issues.

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Whereas satellite measurements of trace gas concentrations and total columns can – in principle – be compared with correlative measurements of similar quantities, space-based remote sensing of particulate matter (PM) in the atmosphere is fundamentally different. The primary parameters derived from satellites are the aerosol optical depth (AOD) and its spectral dependence. AOD is an indicator for the amount of particles in the atmospheric column. The evaluation of particle matter concentrations from AOD data requires some *a priori* knowledge about the vertical profile, the chemical composition and the size distribution of aerosols. This calls for an end-to-end validation of the individual components of the PM data retrieval chain. Furthermore the additional information on aerosol composition and properties is also relevant for the users (e.g., health effects depend directly on the particle size).

2.3.4 Validation of the climate study support services

PROMOTE services supporting climate studies provide global observations of **methane** (CH₄) and **carbon dioxide** (CO₂) **columns** by Envisat SCIAMACHY, as well as multi-satellite measurement records and analyses of vertical **aerosol optical depth** and **speciation** and of **stratospheric aerosols, CH₄ and water vapour** (H₂O). As for other services, the geophysical validation of greenhouse gas (GHG) data is carried out within supporting projects. Relevant projects in the PROMOTE Stage I timeframe were the EC FP5 EVERGREEN and UFTIR, where the retrieval and validation of the targeted trace gases (CO and CH₄) had been addressed, and the ESA-funded project TASTE, providing NDACC-based support to the validation of the Envisat atmospheric chemistry payload. In the PROMOTE 2 timeframe one can cite the EC FP6 HYMN, GEMS and GEOmon, the ESA-funded TASTE and Multi-TASTE, as well as activities relevant to the COST Action WaVaCS (ES0604) and the ISSI WG on Atmospheric Water Vapour.

Correlative data sets appropriate for the validation of satellite-based CH₄ (column and profile) and CO₂ (column) data products are mostly acquired by ground-based FTIR spectrometers affiliated with the NDACC and TCCON networks, although validated column data sets from satellites (EOS-Terra MOPITT and GOSAT TANSO) might also be used. Satellite-based H₂O column data can be validated against NDACC lidars (Raman and DIAL), FTIR spectrometers and microwave radiometers. In the future the use of H₂O column data retrieved from the NOAA Forecast Systems Laboratory (FSL) GPS network might be envisaged as well. NDACC microwave radiometers monitor the stratospheric profile of H₂O at moderate vertical resolution and with a high temporal sampling. Light-weight balloon-borne sensors of different types report the vertical distribution of aerosols (preferably NDACC backscatter sondes) and H₂O (preferably Cryogenic Frost Point Hygrometer (CFH) and Lyman- α sondes, and also Vaisala radiosondes with polymer humidity sensor) from the ground up to the Upper Troposphere/Lower Stratosphere (UTLS). The usability of airborne *in situ* (e.g. MOZAIC and CARIBIC) and of surface *in situ* measurements provided by established networks like ALE/GAGE/AGAGE should be investigated, but here again great care must be given to potential problems raised by differences in sampling and smoothing of atmospheric variability (both temporal and spatial).

While most of GHG services make direct use of satellite measurements, the GHG emission service is based on the inverse modelling technique. Satellite observations are assimilated in 3D chemical transport models and used to infer indirect information on the location and timing of emission sources. For this particular service, validation approaches will be based primarily on comparisons with documented emission inventories. As for

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other assimilation techniques, it must be ensured when validating results of inverse modelling, that the independent observations have not been used at any stage in the inverse algorithms (also not for initialisation or to define statistical behaviour). Interpretation of the validation results regarding emissions should take into account validation results obtained by other services and supporting projects regarding the satellite observations used as input for the inverse modelling of emissions.

2.3.5 Validation of the special services addressing natural hazards

PROMOTE 2 includes several services monitoring consequences of natural hazards to aviation control and public health. While the latter domain has been addressed in the previous section on air quality services (e.g., pollen monitoring and forecast service, and desert dust awareness service), the present section focus on the so-called Support to Aviation Control Service (SACS). SACS is dedicated to the early detection and mapping of abrasive ashes and corrosive sulphur compounds emitted by volcanoes and transported by winds, that represent a major hazard to aviation. The service is to provide in near-real-time satellite-derived data regarding volcanic emissions of sulphur dioxide (SO₂) and of aerosols. In the event of an exceptional SO₂ emission, the service sends an e-mail alert to interested parties, mainly official Volcanic Ash Advisory Centres (VAAC), pointing them to dedicated web pages.

Validation of this two-faceted service should take into consideration the following two tasks: (1) a validation of the individual service components and related geophysical data products, based on classical correlative analysis and information content studies; (2) an evaluation of alert-related aspects. Quantitative validation of SO₂ and aerosol data products of volcanic origin is not straightforward, due to: (1) the difficulty to plan correlative measurement long-term programmes or even campaigns for – nearly – unpredictable eruptions; (2) safety and practical issues to get correlative measurements in the vicinity of an erupting volcano; (3) the current lack of suitable devices to perform accurate SO₂ column measurements from the ground. A major experimental support is provided by the FP6-funded Network for Observation of Volcanic and Atmospheric Change (NOVAC), which operates DOAS instruments at observatories of 15 volcanoes on five continents, including some of the most active and strongest degassing volcanoes in the world. The geographical development of plumes of volcanic ash can be confronted to images provided by satellite instruments like Envisat MERIS and EOS-Aqua MODIS. Aerosol lidars operated in the context of networks like the NDACC and EARLINET can provide correlative information on the vertical structure of the plume and on its temporal development (overpass of station at a given time). Support from (back-)trajectory mapping tools might help the interpretation of correlative studies.

The validation of the SACS starts with its demonstration for a sufficient amount of past volcanic eruptions in long-term satellite data records. The study of alert-related aspects should address the following logical cases (if possible in terms of probability and of detection threshold): (1) a potentially hazardous eruption occurs and SACS does report it; (2) a potentially hazardous eruption occurs and SACS does not report it; (3) a potentially hazardous eruption does not occur but SACS emits an alert. More quantitative analysis might be required, using ground-based SO₂ and aerosol measurements as well as satellite data. Suitable validation methods are still in their infancy and should be further developed.

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3. RESPONSIBILITIES

Responsibilities within PROMOTE 2 are distributed as follows:

- Research partners in charge of algorithm development tasks are responsible for validating individual service components (including new and updated algorithms and their products).
- PROMOTE 2 services line managers supervise the appointment of persons responsible for the validation of individual data products.
- System developers are responsible for the validation against specifications of the services after implementation.
- System providers are responsible for quality assurance against specifications of the services during operations.
- Core users are responsible for the validation against user requirements and for the endorsement of services after implementation.
- The QA/Validation Office is responsible for coordinating the development and enforcement of the *C5 Validation Protocol*, for coordinating the *C6 Service Validation Report*, and for caring for the sustainability of suitable validation information.

It should be pointed out, that core users are expected to play an important role in the validation process through support to the detection of failure of operational services on different levels (production break, quality threshold violation).

The validation of individual service components (new and updated algorithms and their data products) is under the responsibility of the PROMOTE algorithm developers. Since geophysical validation is not an activity directly funded by PROMOTE, results obtained within research or GMES precursor projects of relevance (like e.g. EC FP5-RTD CREATE-DAEDALUS, EVERGREEN, ASSET, UFTIR, DUP-II TEMIS; EC FP6 IP GEMS, HYMN and GEOmon; ESA CHEOPS-GOME, CHEOPS-SCIA, EQUAL, TASTE, Multi-TASTE; EUMETSAT O3M-SAF CDOP; ESA/EUMETSAT Joint EPS/MetOp RAO projects; ESA/NIVR/KNMI Joint OMI AO projects; ...) must be gathered and synthesized. Within each Service Component (and corresponding data product), research partners and service providers collect the available information on the geophysical validation of their respective data products and report to the PROMOTE QA/Validation Office. A key task in the process of collecting validation information is to identify the missing validation information (validation gaps), which is necessary to set priorities for future validation efforts.

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4. QUALITY CONTROL RULES

4.1 Review process and decision sequence

The major steps and responsibilities of the review process are given in figure 2.1 and described in Sections 2 and 3. Through the timeline of a product life cycle, the sequence of decisions to be taken by the responsible for the specific sub-service and the feedback to earlier steps is indicated.

4.2 Long-term quality assurance

This is achieved by relying on the stability of operational archives at the service provider facilities. Thus, data and metadata, as well as quality information, are stored on long term; data loss is prevented by regular control and copying (if necessary) of the files in the archive systems. Data access is provided by their operational catalogue and portal services. The possible use of data mining protocol and processing will be evaluated.

4.3 Principle means of validation


Validation of PROMOTE atmospheric products can rely on comparisons with:

- accurate ground-based, aircraft, and balloon measurements and other satellite observations outside of PROMOTE
- equivalent data products in the service portfolio, already validated or produced by an independent method
- the output of operational atmospheric models with documentary traceability.

4.3.1 Requirements for reference data

In many cases the most accurate validation is done by comparing satellite- and model-based products to well-established reference ground-based, airborne and/or balloon measurements provided by operational networks and by research scientists. These reference correlative data should fulfil several of the following requirements:

- Derived from operational instruments (well-calibrated and monitored; with documented quality standards)
- Well characterised in terms of information content (part of the information contributed by the measurement, as opposed to the part contributed by a climatology, constraints...)
- Instruments at different sites, seasons, daytimes etc. to cover the realistic range of atmospheric states, environmental conditions and measurement scenarios
- With an acceptable level of point-to-area(volume) representativeness (representative for the area under observation in one pixel / one model grid cell)
- Sufficient temporal and spatial resolution to assess the variability scales of the parameters under investigation

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- Long-term observation periods at a few key monitoring sites to assess long-term products (especially the internal consistency of multi-sensor data sets with a view to integrated data use and data fusion)
- Availability within short periods and online for the use in automatic online quality control systems


Generally it is to be assured, that data used for validation have not been exploited during the production process. This logical requirement is not always easy to follow as retrievals can use climatological databases or initialisation data sets generated with the same data. This problem will be critical when a product relies in parts or totally on neural networks and data assimilation tools: the data set used for training the neural network and ingested by the assimilation system should not be – ideally – used for validation purposes.

4.3.2 Requirements for comparison methods

In general, the level of uncertainty due to atmospheric noise on different scales must be taken into account. Remote sensing and models offer only a smoothed/gridded perception of the true three-dimensional atmosphere and its variability. The comparison with other remotely sensed data or modelling results is not straightforward; it must take into account differences in horizontal and vertical resolution, and resulting differences in smoothing and sampling of atmospheric gradients and variability. Neglecting the differences in pixel size / sampling time of point and area observations as well as differences in time and location beyond the variability scale of a parameter can spoil the value of validation. See also Section 2.2.2.2 on the error budget of a comparison.

4.3.3 Equivalent products and model output in the service portfolio


Due to atmospheric variability on various temporal and spatial scales (from the diurnal cycle to decades, from local emissions to global trends) the available amount of ground based measurement data is often not sufficient for a comprehensive validation of atmospheric satellite observations and model results. Therefore, the inter-comparison of equivalent products and of satellite gridded results with model output provides additional statistical information on the consistency of the products. Several parameters are produced as either interim or final products in more than one processing system. This duplication – where it already exists – will not be deleted (due to the large effort in changing the existing decentralized precursor services), but this offers a unique opportunity for quality control: by comparing equivalent data sets from different sensors and algorithms, using standard scoring approaches, the individual product errors and their geographic distribution can be assessed. Furthermore, this provides an additional level of redundancy which can be useful in the case of a failure of one sub-system (e.g. one sensor). In meteorology the so-called “ensemble approach” is a standard approach: several model outputs are treated as a statistical entity to assess the variability of a certain model forecast – this can also be used to better understand the performance of model components in the processing chain.

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4.4 Steps in the validation process

Validation and quality control are conducted at various levels involving the following main steps:

- automatic quality checks (relevance of data range on climatological basis, detection of outliers and aberrant values, compliance with specifications...)
- manual quality control (visual, statistical...)
- scientifically driven geophysical validation of algorithms (end-to-end approach is recommended) and sample products
- statistical quantitative assessment of uncertainties (e.g. bias and precision) of data products in longer time series
- verification and approval of newly implemented service, updates or upgrades
- automatic quality control of operational services wherever possible (depends on available NRT/online reference data)
- monitoring of the performance and reliability of services (e.g. failure rate, distribution delay, data losses)
- assessment of “fitness for purpose” of the service and data products for identified users and usages
- assessment of “fitness for purpose” of the validation carried out to assess the fitness for purpose” of the service and data products; corrective actions in terms of validation plan if needed
- endorsement of a service or data product by the core users
- validation of long-term time series (esp. based on the integration of contiguous data records acquired by different sensors)
- maintenance and distribution of documents (internet, annual summary, document change records, data version records)

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5. STANDARDS

5.1 Maintenance of datasets and reports

One major issue is to ensure long-term safe archiving of atmospheric 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.

Data exchange standards are agreed within the processing chains of the individual sub services of PROMOTE; a generic data exchange protocol for all thematic lines and services is not planned. I/O tools for the formats of end products are provided by several service providers. The choice of formats is facilitated in agreement with core users.


Standards endorsed by European Corporation for Space Standardization (ECSS) are applied whenever possible to assure high quality software. However, given the large amount of existing codes, a reprogramming is not feasible.

5.2 Quality Control metadata and criteria

For each service the provider will collect all relevant information to assess and document the production status and quality of different products (versions). This includes the following types of information:

QUALITY ITEM	DETAILS
Metadata for input data	Acquisition date, processing date, provider, quality flag
Metadata for ancillary data	Version, originator
Processing steps carried out	Algorithms/versions, initialization
Quality results from processing	Warnings, errors
Accuracy assessment (if provided by automatic system or manual control)	Metadata, statistics, quality layer
Data level	Satellite projection, synoptic, assimilated, averaged, ...
Data format including I/O routines	
Documentation	Algorithms, validation

Table 5-1: Summary of major quality control metadata

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Major quality control criteria (which are defined in more detail in the validation plan for each product and service) are:

- On the level of products:
 - Agreement of parameter definition with user requirement
 - Product accuracy (bias, precision, stability or any other relevant expression of uncertainty)
 - Product resolution (horizontal, temporal, vertical)
 - Product visualization
- On the level of services
 - Delivery delay (NRT)
 - Failure rate
 - Data loss rate

5.3 Quality Assurance breakpoints


Intermediate and final products have to be checked for compliance with the defined user requirements. Additionally, the availability of input data for consecutive processing steps and the dissemination of end products at agreed time slots to the defined user interfaces have to be controlled. For this purpose, points in the processing chains, when products are inspected before further processing or delivery (input reception, pre-processing, retrieval, assimilation, post-processing, ...) are defined. This has to be done on a product/service specific level and must be described in the validation report.

5.4 QA and validation documentation

The validation process and its results are recorded as part of the services. Each service provider produces or collects the relevant information and distributes it through the following documents:

- **Validation plans:** Describe the plan for the validation of individual data products and of the service as a whole in all steps described in chapter 2.1, including the sources providing independent reference data.
- **Service Operations reports (S6):** Summarise the behaviour of the services in their operations, including statistical information on stability and data loss.
- **Validation reports (C6):** Integrate all results of validation measures of a respective service from geophysical product and algorithm validation, through validation against specifications and requirements, to the service endorsement.

The *C5 Validation Protocol* (this document) specifies the principles for validation. The validation plans (in principle one for each service) give the detailed plan for validating each product of the service during build-up, operations and update. The validation reports integrate the results for all products of a service until service endorsement. The service operations report summarises the experiences with the service in operations.

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Whereas validation in the build-up phase up to service endorsement is applied one time (with feedback loops if the core user is not satisfied, leading *in fine* to endorsement of the service by the user), the operations reports are published regularly (to be defined per service in the validation plan).

Validation documentation should be published in the open Portable Document Format (.pdf). It must be archived on the long term and should be made accessible to an audience as wide as possible. Validation results will be centralised in the *C6 Service Validation Report* document coordinated and harmonised across services and thematic domains by the Validation Office. Validation-related information (the present *C5 Validation Protocol*, relevant data archives, validation resources, standardisation guidelines, validation manipulations applied, list of supporting projects etc.) will be made available through the web site maintained by the Validation Office. Operations reports and validation reports (after endorsement by the Validation Office) should be delivered via internet portals of the service providers.

5.5 Compliance with international standards and with INSPIRE

The present document evolved with the service portfolio and with users requirements expressed through Service Level Agreements. It also evolved to comply as far as possible with international standardisation requirements formulated e.g. within high-level strategies like the aforementioned QA4EO framework formalised by the 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 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 *C5 Validation Protocol*, 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 will have the more direct application to PROMOTE-like atmospheric services. They will be addressed after 2009, thus after completion of the present project PROMOTE Stage II, but they will impact follow-on projects like MACC, PASODOBLE and EVOSS. Among the relevant themes of Annex III: Atmospheric conditions, Environmental monitoring facilities, Statistical units, Human health and safety, Natural risk zones, Meteorological geographic features. Implications of INSPIRE for PROMOTE Stage II and follow-on activities, as well as the contribution of the PROMOTE Validation Office to the development of IRs, are summarised in document D4 *Service Network – INSPIRE Technical Note*.

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6. TERMINOLOGY

6.1 Abbreviations and acronyms

Preliminary note of best practice: In documents targeting a wide spectrum of potential readers, like validation reports, it is recommended to avoid acronyms and abbreviations except for 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. Using an acronym is acceptable if it has been defined the first time it appears on a page. The same apply to chemical abbreviations. Before using acronyms and abbreviations, authors should keep in mind that it is annoying and difficult – especially in Web-based documents – to turn over several pages in a document to verify the meaning.

ACSG	CEOS WGCV Atmospheric Composition Sub Group
AERONET	Aerosol Robotic Network
AGAGE	Advanced Global Atmospheric Gases Experiment
ALE	Atmospheric Lifetime Experiment
AMF	Air Mass Factor, or optical enhancement factor
AO	Announcement of Opportunity
AOD	Aerosol Optical Depth
ARPA	Regional agency for the protection of the environment (Italy)
ASSET	Assimilation of ENVISAT data
ATSR-2	Along Track Scanning Radiometer 2
BIRA-IASB	Belgian Institute for Space Aeronomy
CARIBIC	Civil Aircraft for Regular Investigation of the Atmosphere Based on an Instrument Container
CDHR	Center for Devices and Radiological Health
CEOS	Committee on Earth Observation Satellites
CMDL	Climate Monitoring and Diagnostics Laboratory (now ESRL)
COST Action	European Cooperation in Science and Technology
CREATE	Construction and use of a European aerosol database
DAEDALUS	delivery of aerosol products for assimilation and environmental use
DIAL	Differential Absorption LIDAR
DLR	German Aerospace Centre
DOAS	Differential Absorption Optical Spectroscopy
DU	Dobson Unit – unit of vertical column density ($2.69 \cdot 10^{16}$ molec.cm ⁻²)
DUE & DUP	ESA's Data User Element & Data User Programme
EARLINET	European Aerosol Research Lidar Network
EC	European Commission
ECSS	European Corporation for Space Standardization
EEA	European Environmental Agency
ENVISAT	ESA's Environmental Satellite, launched on March 1, 2002
EO	Earth Observation
EPA	Environmental Protection Agency
EPS	EUMETSAT Polar System
ERS-2	ESA's Earth Remote Sensing satellite 2, launched on April 21, 1995
ESA	European Space Agency



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ESRIN	European Space Research Institute
ESRL	Earth System Research Laboratory (formerly CMDL)
EVERGREEN	ENVISAT for Environmental Regulation of Greenhouse Gases
EUMETSAT	European Organisation for the Exploitation of Meteorological Satellites
EVOSS	European Volcano Observatory Space Services
FMI	Finnish Meteorological Institute
FP	Framework Programme
FSL	Forecast Systems Laboratory
FTIR(S)	Fourier Transform Infra Red Spectrometer
GAGE	Global Atmospheric Gases Experiment
GAW	WMO's Global Atmosphere Watch
GCOS	Global Climate Observing System
GDP	GOME Data Processor
GEOmon	Global Earth Observation and Monitoring of the Atmosphere
GEO	Group on Earth Observation
GEOS	Global Earth Observation System of Systems
GHG	Greenhouse Gases
GRG	Global Reactive Gases
GMES	Global Monitoring for Environment and Security
GlobAER	Global Aerosol Monitoring
GOME	Global Ozone Monitoring Experiment
GOSAT	Greenhouse gases Observing Satellite "Ibuki"
GPS	Global Positioning System
GSE	GMES Service Element
HYMN	Hydrogen, Methane and Nitrous oxide: Trend, variability, budgets and interactions with the biosphere (EC FP6)
ICSU	International Council for Science
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
IP	EC Integrated Project
I/O tools	Input/Output tools
IR	INSPIRE Implementation Rule
ISO	International Organization for Standardization
ISSI	International Space Science Institute
JAXA	Japan Aerospace Exploration Agency
JCGM	Joint Committee for Guides in Metrology
KNMI	Royal Dutch Meteorological Institute
lidar	light detection and ranging
LUA	North Rhine-Westphalia State Environment Agency
MACC	Monitoring Atmospheric Composition and Climate
MetOp	EUMETSAT's Meteorological Operational satellite
MOPITT	Measurement Of Pollution In The Troposphere
MOZAIC	Measurement of Ozone and water vapour by airbus in-service aircraft
Multi-TASTE	Technical Assistance To the multi-mission validation of Envisat and Third Party Missions using spectrometers, radiometers and sondes
NABEL	Nationales Beobachtungsnetz für Luftfremdstoffe
NDACC	Network for the Detection of Atmospheric Composition Change



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NDSC	Network for the Detection of Stratospheric Change (now NDACC)
NIES	National Institute for Environmental Studies
NOAA	National Oceanic and Atmospheric Administration
NOVAC	Network for Observation of Volcanic and Atmospheric Change
NRT	Near-real time
O3M-SAF	SAF on Ozone and Atmospheric Chemistry Monitoring
ODS	Ozone Depleting Substance
OMI	Ozone Monitoring Instrument
PASODOBLE	Promote Air quality Services integrating Observations – Development Of Basic Localised information for Europe
PBL	Planetary Boundary Layer
PM	Particulate Matter
PROMOTE	GMES Service Element - PROtocol MOniToring for the atmosphere
QA4EO	Quality Assurance framework for Earth Observation
SACS	Support to Aviation Control Service
SAF	Satellite Application Facility
SCIAMACHY	SCanning Imaging Absorption spectroMeter for Atmospheric CHartographY
SGP	SCIAMACHY Ground Processor
SHADOZ	Southern Hemisphere ADDitional Ozonesondes
SLA	Service Level Agreement
SOGE	System for Observation of Halogenated Greenhouse Gases in Europe
SZA	Solar Zenith Angle
TANSO	Thermal And Near infrared Sensor for carbon Observation
TASTE	Technical Assistance To the validation of Envisat using spectrometers, radiometers and sondes
TCCON	Total Carbon Column Observing Network
TEMIS	Tropospheric Emission Monitoring Internet Service
TOGOMI	Total Ozone algorithm for GOME using the OMI algorithm
TOMS	Total Ozone Mapping Spectrometer
TOSOMI	Total Ozone algorithm for SCIAMACHY using the OMI algorithm
UFTIR	Upper free troposphere observations from a European ground-based FTIR network
UNEP	United Nations Environment Programme
UNESCO	United Nations Educational Scientific and Cultural Organization
UVVIS	DOAS UV-visible spectrometer (generic)
VAAC	Volcanic Ash Advisory Centres
VIM	International Vocabulary of Metrology — Basic and general concepts and associated terms
WaVaCS	Water Vapour in the Climate System (COST Action ES0604)
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


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6.2 Terminology

The following terms and definitions have been proposed by standards development organisations of international recognition. They are expected to evolve as these organisations regularly update their standards and as further standardisation and harmonisation occur.


6.2.1 Reference Documents

- [RD7] 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/>
- [RD8] CEOS: CEOS Terms and Definitions, available via <http://calvalportal.ceos.org>
- [RD11] Larssen, S., Sluyter R. and Helmis C. (1999), Criteria for EUROAIRNET – The EEA Air Quality Monitoring and Information Network.
- [RD12] Nappo, C.J., Caneill J.Y., Furman R.W., Gifford F.A., Kaimal J.C., Kramer M.L., Lockhart T.J., Pendergast M.M, Pielke R.A., Randerson D., Shreffler J.H., and Wyngaard J.C. (1982) The Workshop on the Representativeness of Meteorological Observations, June 1981, Boulder, CO, Bull. Am. Meteorol. Soc. 63, 761-764.
- [RD13] NIST: Prokhorov, A. V., R. U. Datla, V. P. Zakharenkov, V. Privalsky, T. W. Humpherys, and V. I. Sapritsky, Spaceborne Optoelectronic Sensors and their Radiometric Calibration. Terms and Definitions. Part 1. Calibration Techniques, Ed. by A. C. Parr and L. K. Issaev, NIST Technical Note NISTIR 7203, March 2005.
- [RD15] 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>


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6.2.2 Recommended terminology

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
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 et al. (1999)
bias	(1) systematic error of indication of a measuring system (2) estimate of a systematic measurement error	VIM
calibration	(1) the process of quantitatively defining the system responses to known, controlled signal inputs (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 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 (2) difference of quantity value obtained by measurement and true value of the measurand	VIM 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

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<i>in situ</i> measurement	(1) a direct measurement of the measurand in its original place (2) any sub-orbital measurement of the measurand	GEOSS
measurand	quantity intended to be measured	VIM
monitoring	systematic evaluation over time of some quantity	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)
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	
random error	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	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 et al. (1982)
reproducibility	measurement precision under a set of conditions including different locations, operators, and measuring systems	VIM
resolution	the least angular/linear/temporal/spectral distance between two identical point sources of radiation that can be distinguished according to a given criterion	NIST

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stability	ability of a measuring system to maintain its metrological characteristics constant with time	VIM
standard uncertainty	measurement uncertainty expressed as a standard deviation	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
uncertainty	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 (2) verification where the specified requirements are adequate for an 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. (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 VIM NIST 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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