Atmospheric Monitoring Services

Stage 2 of the Earthwatch GMES Services Element

PROMOTE 2

C5 Service Validation Protocol

Version 1
Issue 0.2
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<td>J.-C. Lambert (IASB)</td>
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<td>CONTRIBUTING AUTHORS</td>
<td>Authors</td>
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<td>J.-C. Lambert (IASB)</td>
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<td>P. Skarlas (IASB)</td>
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<td></td>
<td>M. Van Roozendael (IASB)</td>
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<td>T. Holzer-Popp (DLR)</td>
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<td>E. Paliouras (DLR)</td>
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<td>F. Baier (DLR)</td>
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<td>K. de Ridder (VITO)</td>
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<td>H. Elber (U. Köln)</td>
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<td>F. Flore (Flyby)</td>
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<td></td>
<td>I. Kilbane-Dawe (CERC)</td>
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<td>A. Mangin (ACRI)</td>
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<td>R. Meerkötter (DLR)</td>
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<td>APPROVED BY</td>
<td>C. Zehner (ESA)</td>
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EXECUTIVE SUMMARY

The second stage of PROtocol MOnitoring for the GMES Service Element (GSE), PROMOTE-2, aims at scaling-up consolidated GMES Services for Atmospheric Monitoring. All services must fulfill quality standards that comply with the users' requirements in terms of needs for further processing or fulfillment of reporting duties on PROMOTE input. Furthermore, the service quality must be kept at a constant level. Appropriate means will be applied during implementation, during operations, and during future updates of the services in order to achieve this quality assurance.

The present Service Validation Protocol document C5 contains 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.

It is to be formally agreed by all members of the service supply partnership, including research partners, operational providers, and system developers. It must also be endorsed by the mandated representatives of the PROMOTE 2 end-user organizations. This includes, as an absolute minimum, all members of the core-user-group.

This document addresses:

- General rules to ensure unbiased and independent validation
- Definition of the tasks of the research partners, system developers, service providers and core users as regards 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
- Approach for validating new products, upgrades, long-term quality assurance, endorsement by key external user-bodies, validation of services (as opposed to products only)
- Requirements for validation documentation
- Document availability, access and distribution rules
- Maintenance of validation standards, reports and data sets.

The service validation protocol builds on more detailed descriptions in technical documents for each product and service, such as validation technical procedures, validation plans, and validation reports.

The validation of each service during its build-up and following updates is fulfilled by a combination of three measures:

- Validation of individual service components
- Validation of products and services against specifications
- Validation of products and services against user requirements.
**DOCUMENT CHANGE RECORD**

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LIST OF ABBREVIATIONS

AERONET  Aerosol Robotic Network
AGAGE  Advanced Global Atmospheric Gasses Experiment
ALE  Atmospheric Lifetime Experiment
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
CMDL  Climate Monitoring and Diagnostics Laboratory
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
DUP  Data User Program
Earlinet  European aerosol research lidar network to establish an aerosol climatology
EC  European Commission
ECSS  European Corporation for Space Standardization
EMPA  Swiss federal laboratory for materials testing and research
ENVISAT  Environmental Satellite
ERS-2  Earth Resources Satellite 2
ESA  European Space Agency
ESRIN  European Space Research INstitute
EVERGREEN  ENVISAT for Environmental Regulation of Greenhouse Gasses
FMI  Finnish Meteorological Institute
FP5  Fifth Framework Program
FTIR  Fourier Transform Infrared Radiometer
GAGE  Global Atmospheric Gasses Experiment
GAW  Global Atmosphere Watch
GDP  GOME Data Processor
GEOMon  Global Earth Observation and Monitoring
GEO  Group on Earth Observation
GEOS  Global Earth Observation System of Systems
GHG  Greenhouse gasses
GMES  Global Monitoring for Environment and Security
GlobAER  Global Aerosol Monitoring
GOA  GOME assimilated and validated ozone and NO2 fields for scientific users and for model validation
GOFAP  GOME Fast delivery and value Added Products
GOME  Global ozone Monitoring Experiment
GSE  GMES Service Element
GUV  Ground based Ultraviolet radiometer
IGOS  Integrated Global Observation System
INSPIRE  Infrastructure for Spatial Information in Europe
I/O-tools  Input/output-tools
ISO  International organization for Standards
<table>
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<th>Abbreviation</th>
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<tr>
<td>LUA</td>
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<td>MOPITT</td>
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<td>MOZAI C</td>
<td>Measurement of Ozone and water vapour by airbus in-service aircraft</td>
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<td>NOVAC</td>
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<td>NRT</td>
<td>Near-real time</td>
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<td>OMI</td>
<td>Ozone Monitoring Instrument</td>
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<td>PBL</td>
<td>Planetary Boundary Layer</td>
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<td>Particulate Matter</td>
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<td>SACS</td>
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<td>SCIAMACHY</td>
<td>SCanning Imaging Absorption spectroMeter for Atmospheric CHartographY</td>
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<td>SHADOZ</td>
<td>Southern Hemisphere ADditional OZonesondes</td>
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<td>SOGE</td>
<td>System for Observation of Halogenated Greenhouse Gases in Europe</td>
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<td>TEMIS</td>
<td>Tropospheric Emission Monitoring Internet Service</td>
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<td>Total Ozone algorithm for GOME using the OMI algorithm</td>
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<td>World Data Center</td>
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<td>WOUDC</td>
<td>World Ozone and Ultraviolet Radiation Data Center</td>
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1. INTRODUCTION

1.1 Purpose

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.

1.2 References

1.2.1 Applicable Documents


[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


[AD8] U7 Service Utility Reports

1.2.2 Reference Documents

1.2.2.1 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


[RD6] U7 Service Utility Reports

1.2.2.2 Service specifications (ATBDs, PSDs...)
1.2.2.3 Validation methods and results provided by Service Networks and by supporting projects

- **[RD7]** Accent, Atmospheric Composition Change, the European Network of Excellence, EU FP6 project, home web page at [http://www.accent-network.org/](http://www.accent-network.org/)

- **[RD8]** AERO-SAM, Boundary layer AEROSol characterization from Space by advanced data Assimilation into a tropospheric chemistry transport Model, DFG-Project (October 2004 – November 2007)

- **[RD9]** AGAGE, Advanced Global Atmospheric Gasses 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/](http://agage.eas.gatech.edu/)

- **[RD10]** ASSET, Assimilation of Envisat data, EU FP5 project, home web page at [http://darc.nerc.ac.uk/asset/](http://darc.nerc.ac.uk/asset/)

- **[RD11]** 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](http://www.enviport.com/cgi-bin/exe.pl?asthma&en&asthma&0)


- **[RD14]** BILRUSIA, Aerosol modelling, Belgian national funded project


- **[RD16]** CHEOPS-SCIA, Climatology of Height-resolved Earth Ozone and Profiling Systems for SCIAMACHY, ESA project

- **[RD17]** COPS, model assimilation of EO & ground-based data (ESA)

- **[RD18]** 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](http://i115srv.vu-wien.ac.at/uv/COST726/Cost726.htm)


- **[RD22]** ENVIRONMENT & HEALTH, long-term high resolution AQ simulation, Belgian national funded project

- **[RD23]** EVERGREEN, EnVisat for Environmental Regulation of GREENhouse gases, EU FP5 project, home web page at [http://www.knmi.nl/evergreen/](http://www.knmi.nl/evergreen/)

- **[RD24]** EXUPERY, SO2 algorithm development for GOME-2, monitoring volcanic plumes, BMBF-Geotechnologien


[RD28] 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

[RD29] MUSTI, Belgian AQ forecast


[RD31] NDMS, Network for the Detection of Mesopause Change

[RD32] NNORSY, Neural Network Ozone Retrieval System

[RD33] NOVAC, Network for Observation of Volcanic and Atmospheric Change, EC-funded project, home page at http://www.novac-project.eu/


[RD36] SA/POLLEN, Finish national funded project


[RD39] SmogProg, AQ forecast, the Netherlands

[RD40] 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/

[RD41] 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/


1.3 Document Overview

This document is organised as follows:

Chapter 1 contains this introduction, including 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 PROMOTE 2 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 validation results, quality control metadata and criteria, quality assurance breakpoints, and documentation.
2. VALIDATION PROTOCOL

2.1 Generic principles

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

Figure 2-1 presents an overview of the major validation tasks to be applied to the PROMOTE 2 service portfolio. From left to right, the box chart shows the timeline for the evolution of service development (top line boxes) through phases from the build-up through operations to updates and its corresponding validation measures/steps (bold boxes in central line). The high level appointment of responsibilities is outlined in the bottom line. It should be emphasized that the build-up of a service is concluded with its formal endorsement by its core users. Furthermore, the most important feedback loops should be highlighted: results from the endorsement process as well as those associated to operations feed back into improvements of algorithms and their operationalisation into services. The following sections describe the major validation tasks in more details.
2.1.1 General principles of validation

The validation of a data product can be seen as a science-driven verification process, the aim of which being to ensure that the data produced (derived from measurements or from model calculations) do respond to expected and predefined quality and information content requirements. Validation generally involves the assessment of the accuracy and precision of the data, over the relevant spatial and temporal domains. The performance of measurement data sets (e.g. satellite observations of column amounts of atmospheric trace gases) must be evaluated through analysis of (1) their agreement with other “reference” measurements of the same quantities (validation of consistency), and (2) their suitability for the targeted geophysical applications (validation of usability).

2.1.1.1 Confrontation with independent reference data

A key aspect in any validation methodology based on comparisons is the selection of correlative data sets, the quality and suitability of which are essential to allow proper unbiased and independent validation. Appropriate 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 general the performance of algorithms will be assessed by comparison with measurements providing the “truth” atmospheric reference. In this case, the principles already stated concerning the selection of correlative data sets apply. However suitable measurements will not always be available, hence validation of data might also involve comparisons with other “reference” model data sets (e.g. results from forecast concentrations can be validated by comparison with later analysis of the same quantities).

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; respective data access agreements 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.

2.1.1.2 Analyses of information content

Although often ignored, a key aspect in the validation of usability (verification of “fitness for purpose”) is the characterization of the information content of the data product. Geophysical quantities retrieved from remote sounding measurements always use 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 really measured information. When a climatology is used in the retrieval, e.g. at altitudes where the measurement is not or less sensitive, 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 *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. 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.

### 2.1.2 Validation of individual service components

Service components are the individual processing blocks by which data products are generated in their interim or final version. The most relevant data products planned for PROMOTE 2 have been 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 summarized in document *C6 Service Validation Report*.

### 2.1.3 Validation against service specifications

Service specifications are outlined in several documents: S5 *Service Portfolio Specifications*, Algorithm Theoretical Basis Documents (ATBDs), Product Specification Documents (PSDs) etc. 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* (SLAs) or recognized from the known use of the data products.

### 2.1.4 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, precision and effective usability of the data product. Such a feedback loop could not be realized 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 will support the different services in establishing a structure linking them to their users in terms of validation.

### 2.1.5 Quality control of services in operations

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.
2.1.6 Validation of service updates

Whenever an update of a service occurs (improved or new algorithm, new sensor, updated photochemical databases), steps 1-3 of the validation in the build-up phase have to be completed: validation of individual components, validation against service specifications, and validation against user requirements. The focus must be logically on expected product changes; nevertheless a verification of the entire processing chain might be required.

2.1.7 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 formalized certification especially when users require this.
2.2 Specifics of validation of the thematic lines

2.2.1 Validation of the ozone services

PROMOTE ozone services provide long time series of observations and NRT analysis/short-term forecasts of the vertical column and profile of atmospheric ozone.

2.2.1.1 Total ozone long-term records

Long-term total ozone records will be derived from observations of known quality by different satellites spanning all together over several decades. The long-term precision and accuracy of existing individual data records have been established through comparison with a large number of ground-based stations from WMO’s GAW and NDACC networks. These results are thoroughly documented in the literature. In comparison to most other PROMOTE data products, total ozone has now reached a high level of maturity. However present requirements are also highly demanding (accuracy high enough to detect a 1% trend per decade) and not easy to fulfill or maintain throughout the entire lifetime of a satellite experiment. Since PROMOTE total ozone records will be generated through the combination of several space-borne instruments (the four successive TOMS, ERS-2 GOME-1, Envisat SCIAMACHY, EOS-Aura OMI, and three MetOp GOME-2), the most challenging aspect of the validation will be to assess trends and the impact of possible bias introduced when integrating these different data sets. Quantification of such bias can be obtained through direct comparison of data sets when overlapping, indirect comparisons using correlative measurements and also using assimilation techniques. A special care must be given to potential effects of differences in ground resolution of the probed information, from 40 x 320 km² for GOME-1 to 17 x 40 km² for OMI.

2.2.1.2 NRT and forecast total ozone

The accuracy requirements on total ozone NRT analysis and forecasts are less demanding than those on long-term data records. On the other hand, timely delivery and resolution of NRT and forecast fields are important issues. Validation of the total ozone forecast data product requires comparisons with high-quality ground-based measurements at selected sites (best maintained Dobson/Brewer stations and UVVIS stations providing NRT data), as well as comparisons with assimilated corresponding analysis. The reliability of the forecasts must be assessed as a function of time and space.

2.2.2 Validation of the UV services

The PROMOTE UV-Products UV-Index and Sunburn time are directly derived (by multiplying with factors) from the erythemally weighted (or weighted by other action spectra) and wavelength integrated UV irradiance in W.m⁻². The product UV-dose is the UV-irradiance integrated over a distinct time interval. Algorithms or models providing UV products use the main UV affecting 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 models, aerosol climatologies) and from algorithms based on geographical and astronomical parameters (solar zenith angle). The accuracy of the observations of atmospheric/environmental parameters like total ozone, cloud
parameters (optical depth and/or coverage), snow coverage and aerosol optical depth directly determines 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.

2.2.2.1 On the level of radiative transfer models

As a preliminary exercise in a validation approach, 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 were inter-compared for a predefined range of the main UV affecting parameters.

2.2.2.2 On the level of UV-irradiance and directly related service 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-irradiances to precise surface measurements (e.g.: spectrally resolved irradiances, UV-A-, UV-B-irradiances, CIE- or other-weighted and integrated irradiances) from well calibrated instruments having documented quality standards. Ideally, local irradiance measurements are complemented with simultaneous measurements of the main UV affecting parameters. Measurements should be performed at different sites (existing stations) representing different environmental conditions (ozone, clouds, snow, elevation, turbidity) and at different daytimes representing an adequate range of different solar zenith angles. The representativeness of local UV measurements should be considered in view of the service specifications that are related to spatial resolution. Accompanying radiative transfer calculations support interpretation and analysis of the results of comparison.

2.2.2.3 On the level of UV doses

With respect to daily doses the main uncertainties are introduced by the diurnal variation of clouds, total ozone and aerosol optical depth. This requires surface measurements of UV-irradiances in a temporal resolution sufficient to represent the diurnal course of these atmospheric parameters. Ideally, simultaneous measurements/observations of UV affecting parameters (clouds, albedo, ozone etc.) are provided in addition to the UV measurements.

An assessment of the accuracy of daily/monthly/seasonal/annual UV-doses needs surface UV-measurements over longer time periods.

The representativeness of local UV measurements should be considered in view of the service specifications that are related to spatial resolution. Accompanying radiative transfer calculations support interpretation and analysis of the results of comparison.

2.2.2.4 On the level of forecasting UV products

The validation of UV-forecast parameters (UV-Indices, sunburn time) requires continuous surface measurements over a defined period at adequately selected sites.
(existing stations) in order to provide data for comparing the forecasted with the actual UV parameters. Temporal resolution and time periods are defined to enable an assessment of the reliability of forecasted parameters as a function of time.

2.2.3 Validation of the air quality services

The PROMOTE air quality monitoring and forecast services generate various kinds of data products (trace gases, aerosols and indices). 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). While regional and local air quality model results can be relatively easily validated using established in-situ network measurements, the geophysical validation of satellite measurements of tropospheric gasses and aerosols is a more challenging task mainly due to:

- the lack or absence of adequate correlative observations
- the large variability (in both time and space) of the atmospheric composition, especially in the vicinity of the earth surface and in regions of strong emissions, which complicates the interpretation of comparison results

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 explicitly account for the known characteristics of the satellite observations (vertical and horizontal resolutions, averaging kernels, time sampling, etc.) as well as those of the correlative measurements. E.g. local high-frequency surface observations of the NO\textsubscript{2} concentration in the planetary boundary layer (PBL) cannot be compared in a straightforward way with tropospheric NO\textsubscript{2} columns derived from GOME scattered-light measurements at its nominal resolution of 40x320 km\textsuperscript{2}. 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 different service components and proper characterisation of the true information content are certainly key issues.

Whereas satellite-based trace gas concentrations and total columns can (in principle) be compared with correlative measurements of similar quantities, space-based remote sensing of particulate matter 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. For its evaluation in terms of particle concentrations knowledge on the vertical profile as well as chemical composition and size distribution of aerosols is required. Furthermore this additional information on aerosol composition is also relevant for the users (e.g. health effects depend on particle size).

2.2.4 Validation of the climate change services

As for other services, geophysical validation of GHG data takes place as part of supporting R&D 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 gasses (CO and CH\textsubscript{4}) were addressed. Correlative data sets appropriate for the validation of satellite-based GHG data products are mostly based on the ground-based
FTIR technique, although airborne in-situ (e.g. MOZAIC) and satellite (current MOPITT, upcoming OCO and GOSAT) data sets might also be used. The usability of in situ measurements provided by networks like ALE/GAGE/AGAGE should be investigated.

For GHG emission service based on the inverse modeling technique where satellite observations are assimilated in 3D chemical transport models and used to infer indirect information on the location and timing of emission sources, validation approaches will be based on comparisons with known emission inventories. As for other assimilation techniques, it must be ensured when validating results of inverse modeling, that the independent observations have not been used at any stage in the inverse algorithms (also not for initialization or to define statistical behavior).

### 2.2.5 Validation of the special services

PROMOTE 2 includes the so-called Support to Aviation Control Service (SACS). SACS is dedicated to the early detection and mapping of abrasive ashes and corrosive sulfur compounds emitted by volcanoes and transported by winds, that represent a major hazard to aviation. The service is to provide in near-real-time data derived from satellite measurements regarding SO\(_2\) and aerosol volcanic emissions and, in the event of an exceptional SO\(_2\) emission, to send an e-mail alert to interested parties, mainly official Volcanic Ash Advisory Centres (VAACs), pointing them to dedicated web pages.

Validation of this two-faceted service should take into consideration the following two tasks: first, a validation of the service components and related geophysical data products, based on classical correlative analysis and information content studies; second, a validation of alert-related aspects. Quantitative validation of SO\(_2\) 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 SO\(_2\) column measurements from the ground. A major experimental support is expected from the FP6-funded Network for Observation of Volcanic and Atmospheric Change (NOVAC), which will operate 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 can provide correlative information on the vertical structure of the plume and on its temporal development (overpass of station at a given time).

In a first stage, the validation of the SACS will be 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 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 might be envisaged in a letter stage, using ground-based SO\(_2\) and aerosol measurements as well as satellite data. Suitable validation methods are still in their infancy and should be further developed.
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 products.
- System developers are responsible for the validation of services after implementation against specifications.
- System providers are responsible for quality assurance during operations against specifications.
- Core users are responsible for validation against user requirements and for the endorsement of services after implementation.
- The 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 products) is under the responsibility of the PROMOTE algorithm developers. Since geophysical validation is not an activity directly funded by PROMOTE, results obtained within related research or GMES precursor projects (like e.g. FP5-RTD CREATE-DAEDALUS, EVERGREEN, ASSET, UFTIR, DUP-II TEMIS, FP6 GEMS, GEMon, ESA CHEOPS-GOME, CHEOPS-SCIA, EQUAL, TASTE…) 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 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.
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. Through the timeline 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 providers facilities. Thus, data and metadata 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 PROMOTE
- equivalent products in the service portfolio, already validated or produced by an independent method
- the output of operational atmospheric models.

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 or balloon measurements provided from operational networks and experts 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 information from the measurement, from a climatology, from constraints…)
- Instruments at different sites, seasons, daytimes etc. to cover the realistic range of environmental conditions
- 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
- Long-term observation periods at few key monitoring sites to assess long-term products (especially multi-sensor data sets with a view to 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 climatologies 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: the data set used for training the neural network should not be – ideally – used for validation.

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 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.

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, 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.

4.4 Steps in the validation process

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

- Manual quality control (visual, statistical)
- Scientific geophysical validation of algorithms and sample products
- Statistical assessment of the accuracy of products in longer time series
- Approval of newly implemented service, updates or upgrades
- Automatic quality control of operational services wherever possible (depends on available NRT/online reference data)
o monitoring of the performance and reliability of services (e.g. failure rate, distribution delay, data losses)

o assessment of “fitness for purpose” for identified users

o endorsement of a service or product by the core users

o validation of long-term time series (esp. based on the integration of contiguous data records acquired by different sensors)

o distribution of documents (internet, annual summary)
5. STANDARDS

5.1 Maintenance of reports and datasets

One major issue is to ensure long-term safe archiving of validation results and metadata needed to qualify the stored products. 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.

ECSS standards 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:

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

Table 5-1: Summary of major quality control metadata

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
  - 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 is 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 validation of products and the service as a whole in all steps described in chapter 2.1 including sources for independent reference data.

- **Service operations reports (S6)**: Summarize 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 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 summarizes the experiences with the service in operations.

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 to endorsement of the service by the user), the operations reports are published regularly (to be defined per service in the validation plans).
Validation documentation should be published in the open pdf format. 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 by the Validation Office. Validation-related information (the present C5 Validation Protocol, relevant data archives, validation resources, standardisation guidelines, 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

It is anticipated that the present document will evolve with the service portfolio and with users requirements expressed through SLAs. An evolution is also foreseen to comply as far as possible with international standardisation requirements formulated e.g. within high-level strategies like the Integrated Global Observation Strategy (IGOS) established by a list of international partners (including CEOS, GAW, GCOS, IGBP, UNEP, UNESCO, WCRP and WMO), or within European initiatives like GMES and INSPIRE (Infrastructure for Spatial Information in Europe). Particular attention will be given to the latter, prepared recently by the European Commission, and aiming at supporting the availability of spatial information for the formulation, implementation and evaluation of Union policies.

END OF DOCUMENT