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DOCUMENT

Requirements for the Geophysical Validation of Sentinel-5 Precursor Products

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1 INTRODUCTION

The Sentinel 5 Precursor (S5P) Mission will form part of the Copernicus Space Component. It is considered as a preparatory project for the next generation, EUMETSAT operated atmospheric composition missions that will comprise both a geo-stationary (Sentinel-4 / part of MTG-S payload) and a polar orbiting (Sentinel-5 / part of MetOp Second Generation payload) component.

Given the planned launch dates of 2019 and 2020 for the first S-4 MTG-S and Post-EPS spacecrafts, respectively, a key role of the S5P mission will be in the provision of atmospheric composition data products covering lower tropospheric pollutants, thus ensuring continuity of the OMI (Aura) mission.

The objective of this document is to define the user requirements for geophysical validation for the S5P mission Phases E1 and E2. It shall, furthermore, provide guidelines for the selection process of the Phase E1 geophysical validation Announcement of Opportunity proposals. The major part of these guidelines will also be applicable to the planning and selection process for the routine geophysical validation activities during Phase E2. The user related issues that need to be tackled by geophysical validation activities are listed in order to identify areas that have not been covered to a satisfactory extent at the end of the geophysical validation proposal review process. Recommendations shall then be made either to adapt some of the geophysical validation proposals or to initiate additional validation activities. Furthermore, the AO proposal review team is asked to check that the proposed validation techniques are appropriate for the purpose of validation of all mandatory and optional space-based data products.

The Sentinel-4/-5 Mission Requirements Traceability Document [R2] describes the mission objectives and scientific requirements of Sentinel-4 and -5 in detail. For S5P the requirements related to S5 are applicable except those requirements that have been addressed in a special section addressing exceptions for S5P, see section 6.7 of [R2].

Focus of this document is product accuracies at Level 2. Level 3 and higher data products may also be validated through comparison with model data, independent satellite measurements and other correlative measurements, the objective being to assess the relative influence of S5P data as compared to other co-located geophysical information.

1.1 Applicable Documents

[A1]	S5P-PL-ESA-SY-166	S5P Commissioning & Cal/Val Implementation Plan (*DRAFT*)
[A2]	S5P-RS-ESA-SY-0002	S5P System Requirements Document (SRD) for Phases B2, C/D, E1

1.2 Reference Documents

[R1]	ECSS system – Glossary of Terms, ECSS-S-ST-00-01C, version: 01 October 2012
[R2]	GMES Sentinels 4 and 5 Mission Requirements Traceability Document, version: 1.0; EOP-SM/2413/BV-bv; 20 September 2012
[R3]	L01B IODS, S5P-KNMI-L01B-0012
[R4]	L01B ATBD, S5P-KNMI-L01B-0009-SD
[R5]	L01B Scientific Quality Requirements Document, S5P-KNMI-L01B-0008-RS
[R6]	Level 2 Input/Output Data Definition - KNMI Products, S5P-KNMI-L2-0009-SD
[R7]	Level 2 Input/Output Data Definition - DLR Products, S5P-L2-DLR-IODD-3002
[R8]	Validation strategy for satellite observations of tropospheric reactive gases, Annals Geophys., 56, FAST TRACK-1, 2013, 10.4401/AG-6335
[R9][1]	TROPOMI ATBD Ozone profile and tropospheric profile; S5P-KMNI-L2-0004-RP; v. 0.9.0
[R10][1]	S5P/TROPOMI Ozone ATBD: part 1 - total column product; S5P-L2-DLR-ATBD-400A; v. 0.9.0 part 2 - tropospheric product; S5P-DLR-IUP-L3-400C; v. 0.9.0
[R11][1]	TROPOMI ATBD of the total and tropospheric NO_2 data products; S5P-KMNI-L2-0005-RP; v. 0.9.0
[R12][1]	S5P/TROPOMI SO_2 ATBD draft; S5P-L2- BIRA-ATBD-400E; v. 0.9.0

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[1] Reference documents [R9] to [R18], i.e. the Level-2 ATBDs, cannot be made available at present as they are undergoing internal review. However, they are not essential for responding to this Call for AO proposals.

[R13][1] S5P/TROPOMI HCHO ATBD draft; S5P-L2-BIRA-ATBD-400F; v. 0.9.0

[R14][1] Carbon Monoxide Columns from the Sentinel-5 Precursor Instrument: ATBD; SRON-S5P-LEV2-RP-002; v. 0.9

[R15][1] ATBD for Sentinel-5 Precursor methane retrieval; SRON-S5P-LEV2-RP-001; v. 0.9

[R16][1] TROPOMI Aerosol ATBD:
part 1 - Aerosol Layer Height Products; S5P-KMNI-L2-0006-RP; v. 0.9.0
part 2 - Aerosol Index Product; S5P-KNMI-L2-0008-RP; v. 0.9.0

[R17][1] S5P/TROPOMI ATBD Cloud Products; S5P-L2-DLR-ATBD-400I; v. 0.9.0

[R18][1] S5P-NPP Cloud Processor ATBD; S5P-NPPC-RAL-ATBD-0001; v. 0.9.0

[R-ISO] International vocabulary of metrology — Basic and general concepts and associated terms (VIM), JCGM 200:2008 (E/F), Joint Committee for Guides in Metrology (http://www.bipm.org/utils/common/documents/jcgm/JCGM_200_2008.pdf)

1.3 Internet References

[R-I1] Copernicus, http://www.copernicus.eu/

[R-I2] Sentinel-4, -5p and -5, http://www.esa.int/Our_Activities/Observing_the_Earth/Copernicus/Sentinels_-4_-5_and_-5P

[R-I3] Copernicus Atmospheric Service, http://www.copernicus.eu/pages-principales/services/atmosphere-monitoring/

[R-I4] MACC-II, http://atmosphere.copernicus.eu/

[R-I5] NDACC, http://www.ndsc.ncep.noaa.gov

[R-I6] TCCON, https://tccon-wiki.caltech.edu/

[R-I7] AERONET, http://aeronet.gsfc.nasa.gov

[R-I8] SHADOZ, http://croc.gsfc.nasa.gov/shadoz/

[R-I9] WOUDC, http://www.woudc.org/

[R-I10] NORS, http://nors.aeronomie.be

[R-I11] EUBREWNET, http://www.eubrewnet.org

[R-I12] NDACC Satellite Group, http://accsatellites.aeronomie.be/index.php/satellite-missions

1.4 Abbreviation List

AAI	Aerosol Absorption Index
AERONET	AErosol RObotic NETwork
AIRS	Atmospheric Infrared Sounder
ALH	Aerosol Layer Height
AO	Announcement of Opportunity
ATBD	Algorithm Theoretical Basis Document
CALIPSO	Cloud-Aerosol Lidar and Infrared Pathfinder Satellite Observation
CARIBIC	Civil Aircraft for the Regular Investigation of the Atmosphere Based on an Instrument Container
CINDI	Cabauw Intercomparison campaign for Nitrogen Dioxide measuring Instruments
Cal/Val	Calibration and Validation
CCI	Climate Change Initiative
CEOS	Committee on Earth Observation Satellites
CKD	Calibration Key Data
DU	Dobson units
EarthCARE	Earth Clouds, Aerosols and Radiation Explorer
ECMWF	European Centre for Medium-range Weather Forecasts
ECV	Essential Climate Variable
ESA	European Space Agency
EUBREWNET	EUropean BREWer NETwork
FOS	Flight Operations Segment
FRESCO	Fast REtrieval Scheme for Cloud from Oxygen A band
FTIR	Fourier Transform Infrared Radiometer
GAW	Global Atmosphere Watch
GDP	GOME Data Processor
GEMS	Geostationary Environmental. Monitoring Spectrometer
GMAP	Geostationary mission for Meteorology and Air Pollution

GODFIT	GOME Direct-FITting
GOME	Global Ozone Monitoring Experiment
GOSAT	Greenhouse gases Observing SATellite
IAGOS	In-Service Aircraft for a Global Observing System
IASI	Infrared Atmospheric Sounding Interferometer
IDAF	Instrument Data Analysis Facility
L1B	Level 1B
L2	Level 2
LEOP	Launch and Early Operation Phase
MACC	Monitoring Atmospheric Composition and Climate
MISR	Multi-Angle Imaging Spectroradiometer
MLS	Microwave Limb Sounder
MAX-DOAS	Multi Axis Differential Optical Absorption Spectroscopy
MERIS	MEdium Resolution Imaging Spectrometer
MOPITT	Measurements of Pollution in the Troposphere
MOZAIC	Measurement of OZone and water vapour on Airbus In-service Aircraft
MTG	Meteosat Third Generation
MTG-S	MTG-Sounder
NDACC	Network for the Detection of Atmospheric Composition Change
NMVOC	Non-Methane Volatile Organic Compounds
NORS	Network Of ground-based Remote Sensing observations
NRT	Near-Real-Time
NWP	Numerical Weather Prediction
OCO	Orbiting Carbon Observatory
OCRA	Optical Cloud Recognition Algorithm
OMI	Ozone Monitoring Instrument
OMPS	Ozone Mapping and Profiler Suite

OSF	Operations Support Facility
PBL	Planetary Boundary Layer
PDGS	Payload Data Ground Segment
ROCINN	Retrieval of Cloud Information using Neural Networks
S-NPP	Suomi National Polar-orbiting Partnership
S5P	Sentinel-5 Precursor
S5PVT	S5P Validation Team
SBUV	Solar Backscatter UltraViolet instrument
SHADOZ	Southern Hemisphere ADditional OZonesondes
SWIR	ShortWave InfraRed
TCCON	Total Carbon Column Observing Network
TEMPO	Tropospheric Emissions Monitoring of POllution
TES	Tropospheric Emission Spectrometer
TM	Telemetry
TTC	Telemetry, Tracking & Command
TROPOMI	TROPOspheric Monitoring Instrument
UVN	Ultraviolet Visible Near-Infrared
VIIRS	Visible/Infrared Imager Radiometer Suite
WMO	World Meteorological Organisation
WOUDC	World Ozone and Ultraviolet Radiation Data Centre

2 DEFINITIONS

The following definitions are applicable to this document:

Accuracy:
Closeness of agreement between a measured quantity value and a true quantity value of a measured parameter [R-ISO].

Calibration:
The process of quantitatively defining the system responses to known, controlled signal inputs (CEOS Definition).

Generally, *calibration* shall comprise all operations for the purpose of determining the values of the errors and, if necessary, other metrological properties of a measuring instrument.
In the context of this document '*calibration*' shall be the process of transforming data represented in arbitrary or instrument specific ('engineering') units into physically meaningful units.

Characterisation:
'Characterization' represents a set of measurements of a specific quantity under well-defined, variable conditions. The purpose of a characterization is to allow the assignment of an expected result valid at a later instant, given the exact conditions valid at that instant and the results of the characterization measurements.

Precision:
Closeness of agreement between measured quantity values obtained by replicate measurements on the same or similar objects under specified conditions. Precision is usually expressed numerically by measures of imprecision, such as standard deviation, variance, or coefficient of variation under the specified conditions of measurement [E-ISO].

Validation:
The process of assessing, by independent means, the quality of the data products derived from the system outputs (CEOS Definition).

Validation may also refer to an algorithm used for on-ground data processing, or a part thereof. In this case *validation* is the sum of tests performed on that component under variable conditions, with the purpose of assessing its overall performance with respect to numerical accuracy, impacts of modelling/approximation errors and sensitivity to measurement or auxiliary input data errors

Verification:
Provision of objective evidence that a given item fulfils specified requirements [R-ISO].

Phase E1:

The commissioning phase. In the case of S5P this period will cover the initial 6 months of in-flight operation. Within this period platform and instrument will be switched on and functionally checked out. In addition, the instrument will be characterized and a routine in-flight calibration scenario will be established.

Phase E2:
The operational phase of the S5P satellite. In this phase, any instruments are assumed to operate in a stable measuring mode. Routine instrument calibration is performed. Only smaller changes to the instrument settings, measurement modes, and algorithm updates are expected.

Level 0 Data :
Raw, unprocessed instrument measurement data (atmospheric and calibration modes) in all TROPOMI spectral bands, housekeeping data; data files sorted by instrument mode / application process.

Level 1a Data:
Reconstructed unprocessed data at full resolution, time referenced, and annotated with ancillary information, including radiometric and geometric calibration coefficients and geo-referencing parameters (e.g. ephemeris) computed and appended but not applied to the Level 0 data.
(provided for completeness only as Sentinel-5p does not have such a product)

Level 1b Data:
Calibrated, geo-located Earth reflectance and radiance spectra in all spectral bands; solar irradiance data, annotation data and references to used calibration data.

Level 2 Data:
Derived geophysical parameters at the same resolution and location as Level 1 source data.

Level 3 Data:
Data or retrieved geophysical parameters which have been spatially and/or temporally re-sampled (i.e. derived from Level 1 or 2 products), usually with some completeness and consistency. Such re-sampling may include averaging and compositing.

Level 4 Data:
Model output or results from analyses of lower level data (i.e. parameters that are not directly measured by the instruments, but are derived from these measurements).

(Level 3 and Level 4 definitions are only provided for completeness)

3 MISSION OVERVIEW

3.1 The Copernicus Framework

Copernicus [R-I1] is the European system for monitoring the Earth.

Copernicus consists of a complex set of systems, which collect data from multiple sources: Earth observation satellites and in situ sensors such as ground stations, airborne and sea-borne sensors. It processes these data and provides users with reliable and up-to-date information through a set of services related to environmental and security issues.

The services address six thematic areas: land, marine, atmosphere, climate change, emergency management and security. They support a wide range of applications, including environment protection, management of urban areas, regional and local planning, agriculture, forestry, fisheries, health, transport, climate change, sustainable development, civil protection and tourism.

The main users of Copernicus services are policymakers and public authorities, who need the information to develop environmental legislation and policies or to take critical decisions in the event of an emergency, such as a natural disaster or a humanitarian crisis.

Based on the Copernicus services and on the data collected through the Sentinels and the contributing missions, many value-added services can be tailored to specific public or commercial needs, resulting in new business opportunities. In fact, several economic studies have already demonstrated a huge potential for job creation, innovation and growth.

The Copernicus programme is coordinated and managed by the European Commission. The development of the observation infrastructure is performed under the aegis of the European Space Agency for the space component and of the European Environment Agency and the Member States for the in situ component.

3.2 Spacecraft & Payload

3.2.1 The Sentinel-5 Precursor Spacecraft

The Sentinel 5 Precursor (S5P) mission is a low Earth orbit polar satellite system to provide information and services on air quality, climate and the ozone layer in the timeframe 2015-2022 [R-I2]. The S5P mission is part of the Copernicus space component programme. It consists of a satellite bus, the TROPOspheric Monitoring Instrument (TROPOMI) payload, and the ground segment. In this section a description of the mission is provided with emphasis on those aspects that are relevant for the geophysical validation of the S5P products. A comprehensive description of the mission can be found in [R2] and [A2].

The orbit definition of the S5P mission plays an important role in the operational aspects. Both instrument operations and data processing use a coordinated orbital scenario. This orbital scenario is also linked to in-flight calibration of the instrument. S5P will fly a sunsynchronous polar orbit, in so-called close formation with the NOAA/NASA Suomi-NPP (S-NPP) mission. Loose formation means that the difference in overpass time between S5P and S-NPP will be less than 5 minutes. The main driver for the formation flying is the cloud clearing for the CH_4 product using the high spatial resolution data from the Visible/Infrared Imager Radiometer Suite (VIIRS), but additional synergies are expected.

The orbital parameters for S5P are given in Table 1.

Table 1: Parameters of the S5P reference orbit.

Operational parameters	**Value**
Repeat Cycle	16 days
Cycle Length	227 orbits
Semi-Major Axis	7202.1625 km
Eccentricity	0.001
Inclination	98.7 deg
Argument of Perigee	90.00 deg
Mean Local Solar Time of Ascending Node Crossing	13:35 hrs +/- 5 minutes
Orbital period	6090 s

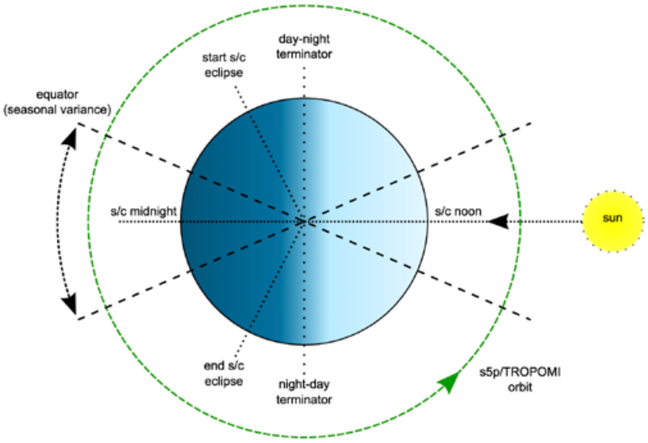

Figure 1: S5P orbit overview.

Each S5P orbit has a day (sun-lit) side and a night (dark) side (See Figure 1). On the day-side the spacecraft flies from south to north; on the night side it flies from north to south. Spacecraft midnight is defined as the time halfway the nadir day-night terminator and the nadir night-day terminator; spacecraft noon is the time halfway the nadir night-day terminator and the nadir day-night terminator. Both the instrument operations as well as data processing will use the spacecraft midnight as the start and end points of an orbit.

This convention has the advantage that the orbits are defined without any seasonal dependency. Due to seasonal variation, the position of the equator with respect to the spacecraft midnight will change. As a result, spacecraft midnight is not at a fixed latitude.

3.2.2 The Sentinel-5 Precursor Payload TROPOMI

The payload of the S5P mission is TROPOMI that will measure the nadir atmospheric spectra at a high spectral resolution in the UV-Visible, NIR and SWIR bands. Key atmospheric constituents, including ozone (O_3), nitrogen dioxide (NO_2), sulphur dioxide (SO_2), carbon monoxide (CO), methane (CH_4), formaldehyde (HCHO) as well as cloud and aerosol properties, can be derived from the observations. TROPOMI is a push broom imaging spectrometer with a wide field of view that provides daily global coverage with high spatial resolution. The measurement principle of TROPOMI is illustrated in Figure 2.

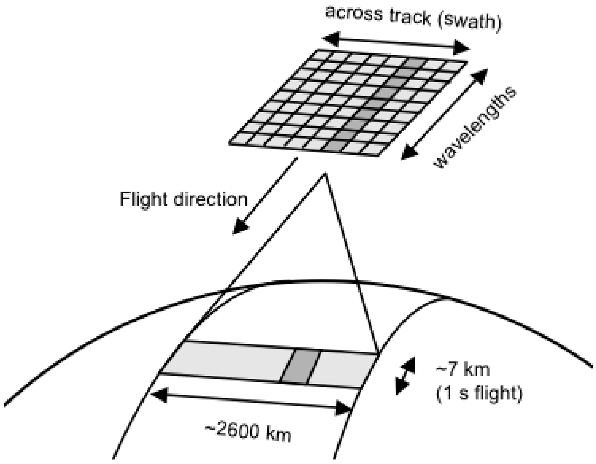

Figure 2: TROPOMI measurement principle. The dark-grey ground pixel is imaged on the two-dimensional detector as a spectrum. All ground pixels in the 2600 km wide swath are measured simultaneously.

The instrument images a strip of the Earth on a two dimensional detector for a period of one second during which the observed swath satellite moves by about 7 km over the Earth's surface. This strip has dimensions of approximately 2600 km in the direction across the track of the satellite and 7 km in the along-track direction. After the 1 second measurement a new measurement is started. In this way, the instrument scans the Earth as the satellite moves. The two dimensions of the detector are used to detect the different ground pixels in the across track direction and for the different wavelengths. The collected light is separated in the different wavelengths using grating spectrometers. TROPOMI has four spectrometers, covering non-contiguous wavelength bands from the ultraviolet to the shortwave infrared.

3.3 Ground Segment

The S-5P ground segment will be in charge of the overall commanding and monitoring of the spacecraft as well as the acquisition, processing and dissemination of observational data. The corresponding primary components, the Flight Operations Segment (FOS) and the Payload Data Ground Segment (PDGS) will be developed under separate contract activities, under overall ESA responsibility, see Figure 3.

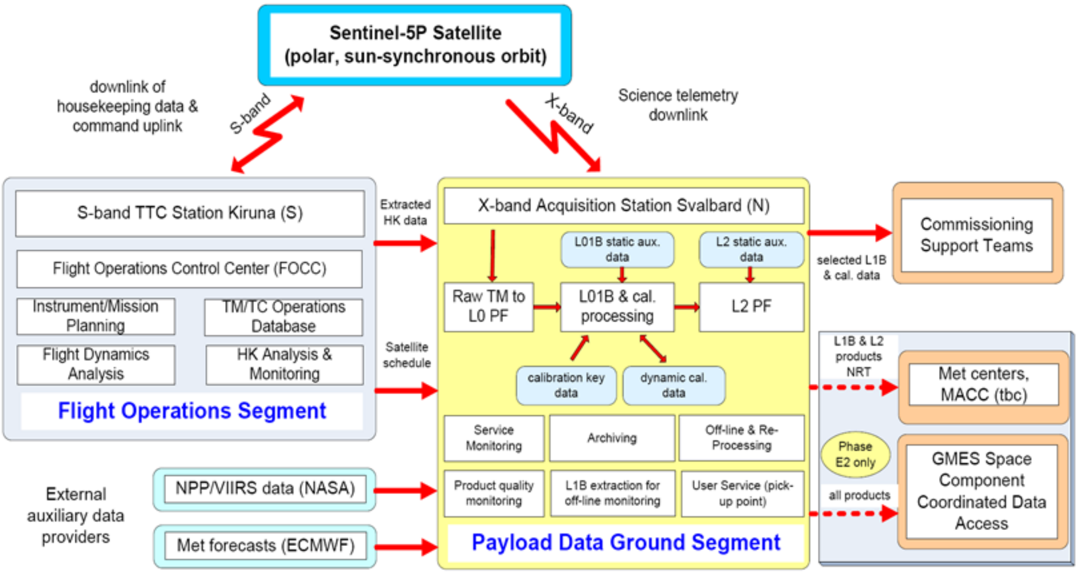

Figure 3. The Sentinel 5 Precursor Ground Segment (schematic view)

3.3.1 *Flight Operations Segment (FOS)*

The **FOS** will comprise the following elements:

- The ESA operated S-band Telemetry, Tracking & Command (TTC) station in Kiruna (Sweden),
- additional TTC stations as required during the Launch and Early Operation Phase (LEOP),
- the S5P Mission Control System,
- the S5P Mission Planning System (covering spacecraft operations & TROPOMI instrument planning as well as S-/X-band downlink scheduling),
- a S5P System Simulator, for testing of the MCS, database validation and FOS system level validation and training,
- interfaces to the PDGS for the reception of S-/X-band ground station availability information,
- an interface to the TROPOMI Operations Support Facility (OSF) at KNMI for the reception of planning related data required for the operation of the TROPOMI instrument, and for the delivery of TROPOMI schedule data,
- interfaces to industry and to ESA external expert teams for the delivery of extracted house-keeping /engineering telemetry,
- an interface to industry for the reception of on-board software maintenance data,
- additional facilities related to the Flight Dynamics, Ground Station operation, monitoring and planning tasks.

3.3.2 *Payload Data Ground Segment (PDGS)*

The **PDGS** will comprise the following elements:

- An interface to the S-/X-band Acquisition Stations in Svalbard (N) and complementary acquisition stations for the reception of raw telemetry data ('science' TM),
- a Level 0 to Level 1B Processing Facility performing routine near-real-time and off-line processing tasks for TROPOMI atmospheric and calibration measurements and related quality control tasks,
- Level 2 (L2) Processing Facility, hosting the various processors for the generation of near-real-time and off-line S5P geophysical data products, as well as basic quality control functions
- an interface for the delivery of S-/X-band station availability and station use data to the FOS,
- exchange of planning data between the TROPOMI Operations Support Facility at KNMI and the FOS,
- an interface for the reception of externally provided auxiliary data (S-NPP cloud mask data, Met forecasts, ...),
- an interface to the Instrument Data Analysis Facility (IDAF), for the delivery of subsets of Level 1B / Level 2 data and the reception of Calibration Key Data (CKD), TM5 profile data and L2 off-line data sets,
- a pick-up point for the delivery of L1B / L2 data products to commissioning & Cal/Val support teams during Phase E1,
- an Archiving Facility, for short- and medium-term archiving of all generated data products,
- an interface to the Copernicus Coordinated Data Access infrastructure, to support user service and product dissemination tasks (only required during Phase E2),
- a Reprocessing Facility.

3.4 Operation Concept

3.4.1 *Payload operation*

The S-5P mission concept is based on the routine operation of the TROPOMI instrument in nominal measurement mode performing either measurements of the atmospheric scene or calibration activities. Whereas atmospheric radiances measurements will be nominally performed on the day-side part of the orbit background image measurements will be acquired during each eclipse period.

Solar irradiance measurements (i.e., measurements of the top-of-atmosphere reflectance) will be commanded approximately once every 15 orbits. Various additional calibration activities, including measurements of internal white light and spectral line sources will be scheduled periodically. All data will be recorded in the on-board mass memory and dumped during regular ground station passes.

During early in-orbit operation (Phase E1) frequent updates to scheduled calibration activities and to the instrument settings will occur. However, during routine operation (Phase E2) the mission planning of S5P will be based on a stable orbit scenario ('background mission'), with periodic execution of TROPOMI calibration and atmospheric target measurements in line with an instrument specific cycle of 360 orbits / 24 days.

3.4.2 Ground communication

The Sentinel-5P spacecraft provides separate communication channels

- an S-band link, used for telecommanding, tracking tasks and for the downlink of housekeeping telemetry
- an X-band link for the downlink of 'science' telemetry, i.e. TROPOMI observational data and related engineering telemetry.

Whereas the ESA ground station in Kiruna (Sweden) is used for spacecraft commanding and monitoring tasks (S-band) the acquisition station Svalbard (Norway) will be used for periodic dumps of recorded S- and X-band telemetry. Use of Inuvik (Canada) as complementary acquisition station is envisaged to reduce the latency for TROPOMI measurement data between sensing and availability at the Payload Data Ground Segment (PDGS). Use of the dual station downlink scenario will ensure the near-real-time (NRT) dissemination service envisaged for global Level-2 data products will be achieved.

3.5 Sentinel-5 Precursor Products

Table 2 provides an overview over the species that shall be considered in the context of the Sentinel-5P mission split into mandatory and optional products. The primary focus of validation call is on the mandatory products. However, proposals for validation of optional products are welcome.

Table 2: Sentinel-5 Precursor products.

	Total Column	Tropospheric Column	Profile
Mandatory Products			
Ozone - O_3	Yes	Yes	Yes
Nitrogen dioxide - NO_2	Yes	Yes	No
Sulphur dioxide - SO_2	Yes	No	No
Formaldehyde - HCHO	Yes	No	No
Carbon monoxide - CO	Yes	No	No
Methane - CH_4	Yes	No	No
Aerosols *(aerosol index, layer height)*	Yes		
Clouds *(fraction, optical depth, layer height)*	Yes		
Optional Products			
Surface UV	Yes		
Aerosol Optical Depth AOD	Yes		
Water vapour - H_2O	Yes	No	No
Glyoxal – CHOCHO	Yes	No	No
Bromine monoxide - BrO	Yes	No	No
Chlorine dioxide - OClO	Yes	No	No
Deuterated water/water ratio - HDO/H_2O	Yes	No	No

Related to the products are requirements about accuracy split into bias and random. They have been summarised in Table 3.

Table 3: Sentinel-5 Precursor Product Accuracies split into bias and random for the mandatory products.

Product Group	***Data Product***	***Vertical Resolution***	***Bias***	***Random***
Ozone	Ozone Profile	6 km	10-30%	10%
	Total Ozone	total column	6%	1.6%
	Tropospheric Ozone	trop column	25%	10%
NO_2	Stratospheric NO_2	strat column	<10%	0.5e15
	Tropospheric NO_2	trop column	25-50%	0.7e15
SO_2	SO_2 enhanced	total column	30-50%	0.5 (0.2) DU
	Total SO_2	total column	30-50%	0.5 (0.2) DU
CH_2O	Total CH_2O	total column	40-80%	1.2e16 (4e15)
CO	Total CO	total column	15%	<10%
CH_4	Total CH_4	total column	1%	1%
Aerosol	Aerosol Type	total column	~1 AAI	<0.1 AAI
	Aerosol Layer Height	total column	<100hPa	<50hPa
Cloud	Cloud Fraction	total column	20%	5%
	Cloud Height (Pressure)	total column	<0.5 km (100hPa)	<0.3 km (50hPa)
	Cloud Optical Thickness	total column	20%	5%
Irradiance	Spectral UV solar irradiance	n/a		
	Surface UV	n/a	TBD	TBD

A Mission Performance Centre responsible for the assessment of the operational product content quality as well as the evolution of the processing baseline will be established for Phase E2.

4 VALIDATION NEEDS

4.1 The Validation Challenge

The main target of S5P is to provide information and services on air quality, climate and the ozone layer. In the past two decades, a validation community has been established focussing on the validation of products related to the ozone layer. In this frame, dedicated measurement systems and networks were developed along well-established validation procedures and routines.

In contrast to the stratosphere, the validation of tropospheric reactive trace gases poses a number of additional challenges [R8]. They have a high variability in time and space, both horizontally and vertically. As a result their distribution is characterised by strong gradients. Many species are influenced by an active photochemistry leading to diurnal variations. Their distribution is strongly depending on local emission sources. The retrievals are depending critically on the a-priory information, which needs to be well controlled along with the products themselves. Further, their tropospheric signal is small either due to the low concentration or the relative abundance with respect to the stratosphere. The retrievals themselves are complex and the a-priori assumptions and individual steps need to be assessed through the validation of input and intermediate products. This list, which does not claim to be complete, illustrates a necessary change in validation paradigm.

The validation activities proposed in the call need to clearly indicate how they address the challenges for the tropospheric products.

4.2 Initial in-flight validation needs (Phase E1)

The functional verification of the TROPOMI instrument and of the related ground processor components are essential tasks during early in-orbit operation. These tasks will largely base on the analyses of calibration and characterization measurements acquired in flight and of generated Level 1B products and related monitoring parameters.

In view of the higher level processing tasks and of a correct interpretation by the end users an accurate assessment of end to end error budgets of geophysical products is essential. This will cover the following aspects in particular:

- an initial assessment of error budgets in Level 1B and 2 products,
- a selection of sources of information allowing an independent assessment of the overall quality of generated products,
- comparisons of key geophysical parameters with independent measurements correlated in time and space with TROPOMI observations,
- the verification of the consistency between geophysical parameters derived from TROPOMI and correlative measurements within the error budgets assigned to each data set.

It is assumed that the validation of Sentinel-5P data products will not be restricted to direct comparisons between TROPOMI and correlated measurements but may also comprise checks of its data products against modelled data and the results of assimilation experiments.

4.3 Long-term validation needs (Phase E2 to LTDP)

Given the very limited time frame of the commissioning phase and the expected need to evolve the Level 1b and Level 2 processors, the validation efforts need to be continued into the operations Phase E2. This shall allow a comprehensive assessment of the S5P product quality, including the validity and the stability throughout the instrument operation, during the post-operation period (Phase F) as well as for the Long Term Data Preservation, if required.

The activities shall allow a continuous, long-term

- provision of consolidated product quality information in terms of accuracy and precision estimates to the Copernicus services and science community,
- support to the processor developments by validation of algorithm error estimates as well as intermediate products, auxiliary information, incl. databases, and basic assumptions,
- assessment of validation needs,
- monitoring of the instrument characteristics.

The long-term validation activities build on operational, or quasi-operational, ground based validation capabilities, validation campaigns and models.

5 APPLICATIONS & END USERS

In the frame of the Copernicus Sentinel missions several user typologies are identified. The primary users of the data are the Copernicus Operational Services. S5P will mainly support the Atmospheric Service, but support to other services like the Climate Service is possible. Other users types include the scientific community, ESA member states through collaborative ground segments, public and commercial value adding entities as well as support to international agreements.

5.1 Copernicus Atmospheric Service

The Copernicus Atmosphere monitoring service [R-I3] provides continuous data and information on atmospheric composition. The service describes the current situation, forecasts the situation a few days ahead, and analyses consistently retrospective data records for recent years.

The Copernicus atmosphere monitoring service supports many applications in a variety of domains including health, environmental monitoring, renewables energies, meteorology, and climatology. It provides daily information on the global atmospheric composition by monitoring and forecasting constituents such as greenhouse gases (carbon dioxide and methane), reactive gases (e.g., carbon monoxide, oxidised nitrogen compounds, sulphur dioxide), ozone and aerosols.

The Monitoring Atmospheric Composition and Climate-II (MACC-II) [RI4] is the pre-operational implementation of the service and currently provides access to:

- Global Reanalysis (2003 - 2012) for aerosol, reactive gases, greenhouse gases
- Global near-real-time analyses and 5-day forecasts for aerosol and reactive gases
- Near-real-time analyses and forecasts of stratospheric ozone and related species from IFS-MOZART, BASCOE, SACADA, and TM3DAM models
- Total ozone multi-sensor reanalysis (1978 - 2009)
- Near-real-time global 5-day forecasts of UV index
- Near-real-time global forecasts of CO_2 at high resolution (16km)
- Delayed-mode analyses of aerosol and greenhouse gases at high resolution (40km)
- Reanalysis of global carbon dioxide surface fluxes (1979 - 2012)
- Reanalysis of global methane surface fluxes (2003 - 2011)
- Delayed-mode surface fluxes of carbon dioxide, methane, and nitrous dioxide
- Reanalysis of aerosol direct forcing (2003 - 2012)
- Reanalysis of aerosol indirect forcing (2003 - 2012)
- Stand-alone retrieval of methane from SCIAMACHY (2003 - 2012)
- analyses and 4-day forecasts of key atmospheric pollutants (ozone, NO_2, SO_2, PM2.5, PM10, CO, etc.) in the form of maps and numerical data from the individual forecast systems and from the European ensemble built upon these;
- products tailored to meet users' common general needs (integrated AQ indicators, surface maps indicating probability of exceeding certain air quality thresholds, etc.);
- seasonal pre-operational birch pollen forecasts;
- verification results in the form of maps and time-series over the sites that regularly report observed values;
- European Air quality evaluation reports;
- McClear clear-sky surface solar radiation
- RAD-SOLAR archive of surface solar irradiance
- Country source-receptor calculations
- Regional source-receptor calculations
- Green scenario toolbox

The Monitoring Atmospheric Composition and Climate-II (MACC-II) [RI4] is the current pre-operational implementation of the service.

5.2 Scientific End Users

Science has been identified as a major user of the Sentinel, and in particular of S5P, data. Due to the long instrument heritage in Europe, ranging back to GOME on ERS-2, a broad and vibrant research community has developed and will exploit the products provided by S5P. Major improvements for Copernicus Services and the value adding industry, but also for the S5P mission and its products, are expected to result from the science activities supported by the EC, National Agencies or ESA.

It is expected that Scientific End Users will receive measurements that require no further processing, i.e., Level 1b and Level 2 data, for their application and which are supported by estimates of their uncertainty.

6 VALIDATION OVERVIEW

6.1 Commissioning Phase Overview

The Commissioning Phase will cover the initial 6 months period of Sentinel-5 P in-orbit operation. This period is dedicated the execution of a set of functional tests in order to verify the overall health of the satellite and the performance of the various sub-systems, including the TROPOMI payload instrument.

The S5P mission tasks during Phase E1 will include

- Launch and Early In-Orbit Operation Phase (LEOP), including the orbit injection, solar array deployment and acquisition of nominal attitude
- In-Orbit verification and spacecraft commissioning, covering

    - platform equipment switch on and functional check-out (commanding, data handling, downlink, ...)
    - TROPOMI de-contamination & switch-on (approx. 4 -6 weeks after launch)
    - check-out of instrument sub-systems, verification of instrument health and conduct of instrument specific calibration tasks
    - acquisition and monitoring of TROPOMI HK telemetry & updating of configuration settings

- initialization of on ground planning, data circulation & processing tasks
- processing of in-flight calibration and atmospheric scene data
- optimization of periodic in-flight calibration scenarios (settings, calibration cycles ..)
- functional verification of the Level 1B and Level 2 algorithms and optimization of configuration data
- support of early Calibration and Validation (Cal/Val) activities
- deployment of full functionalities of the S5P Ground Segment in preparation the Phase E1-E2 handover.

6.2 Routine Operations (Phase E2)

During Phase E2, S5P will be operated in a nominal routine operational mode according to the Phase E mission operational plan. Activities include the operational control of the satellite and instrument health and safety, mission planning and orbit control, system performance assessment, as well as the on-ground data acquisition, processing, calibration, distribution, archiving and assessment of product quality.

S5P data will be provided to the Copernicus services, in particular the Atmospheric core service, the science community, value adding entities and the Member States via well-defined user interfaces. A mission performance centre, consisting of expert teams, will be responsible for the assessment of the product content quality as well as the evolution of the processing baseline. Upon major updates, reprocessing campaigns for a selection or all S5P products are envisaged.

During Phase E2 the routine end-to-end performance assessment needs to be supported by continuous validation activities ensuring a traceable data quality. In addition, for major changes in the processor or product baseline, e.g., new products or major reprocessing campaigns, dedicated validation activities will be needed to assess the data against its requirements.

6.3 Post Operation Phase (Phase F)

The post operation phase (Phase F) ends with the decommissioning and disposal of the S5P satellite. Except for monitoring of the satellite position by passive means, all space segment activities will terminate. PDGS tasks related to the product evolution will be ramped down according to the needs of Copernicus Services and other users, and the available resources. Validation activities will support potential baseline evolution and reprocessing activities.

6.4 Long Term Data Preservation (LTDP)

The aim of the LTDP is to ensure and facilitate the accessibility and usability of the preserved data sets for an unlimited time span following the completion of all Phase F tasks. Further data exploitation activities will be defined in another, not S5P mission related, framework.

7 VALIDATION REQUIREMENTS

7.1 General Requirements

The general purpose of the calibration and validation of S5P data is to provide confidence in estimates of the uncertainties. In principle, this may be determined by examining the difference between the different data products and a suitably large number of independent, accurate measurements. In practice such a scheme is scarcely available and if it would be available there would be limited point in flying the satellite.

Therefore a sensible approach is needed to characterise the temporal and spatial scale of the uncertainties. Since the validation requires a wide range of atmospheric measurements a certain set of requirements are needed for these in order to optimally make use of existing resources and implement new measurements via airborne or ground-based campaigns or other more long term activities to address existing gaps.

The product specific requirements described below assist this process by describing:

- A framework for the key parameters of the different products together with a treatment of requirements and their breakdown into components.
- The expected nature of uncertainty in the S5P measurements and their likely temporal and spatial scales.
- The Representativeness of observations (space and time); at the basic sampling scale.

In addition the experiments, sensors, platforms and correlative measurements that may most usefully estimate the uncertainties are described per data product.

7.2 Product Specific Requirements for Mandatory Products

7.2.1 Ozone (O_3)

From TROPOMI/S5P the following ozone products will be derived:

- total ozone column;
- ozone profile;
- tropospheric ozone column.

For the ATBD references, see [R9 and R10].

7.2.1.1 Total ozone validation

Comprehensive validation campaigns for GOME/ ERS-2 total ozone data have been carried out during the last two decades, see for example the validation of the official products generated with GDP 4.0 and GDP 5. The GDP 4.x algorithm has also been validated for Sciamachy/ENVISAT, and GOME-2 data from MetOp-A and MetOp-B. The main emphasis is on quality assessment of retrieved ozone column amounts on a global scale and over long time periods. The validation exercise should establish whether total ozone data quality meets the requirements of most demanding geophysical research applications like long term trend monitoring on the global scale, polar process studies, and research on ozone-climate interactions. In addition, the validation should investigate the consistency between GOME-type total ozone data and ozone data records from other satellites, using ground-based networks as a standard transfer.

For previous missions, validation studies have been based on comparisons with correlative observations acquired by ground-based reference instruments contributing to WMO's Global Atmosphere Watch (GAW), namely, Brewer and Dobson ultraviolet spectrophotometers (World Ozone and Ultraviolet Radiation Data Centre, WOUDC) and DOAS UV-visible spectrometers (NDACC). In this regard, the GDP 5 GOME-data validation is perhaps the most instructive and far-ranging. This includes an inter-comparison of GDP 4.0 and GDP 5 against the Dobson and Brewer networks.

In addition to comparison with the ground-based networks, intercomparison between different European satellite missions, including the Sciamachy period (2002-2012), the GOME period (1995-2011), GOME-2 (2007 to present), and OMI (2004 to present), as well as USA missions like SBUV and OMPS are important to establish the accuracy of the long-term data record.

7.2.1.2 Ozone profile validation

The ozone profile product from S5P will have typical vertical resolution of 6-7 km, with about one piece of information in the troposphere. For correlative ozone profile data sets used for the validation of this product, it is essential to have a higher vertical resolution and less dependence on a-prior information. Because there are no correlative data sets that fulfil this requirement from the surface to the higher stratosphere, validation will depend on multiple correlative datasets, including balloon sounding, LIDARs as well as satellite intercomparisons. Comparisons with limb viewing instruments (e.g., MLS, OMPS) are important, mainly to validate stratospheric ozone. Such comparisons have the advantage of providing global coverage and much more statistics, as compared to balloon soundings. Infrared instruments such as Tropospheric Emission Spectrometer (TES) and Infrared Atmospheric Sounding Interferometer(IASI) could be used to compare the tropospheric column.

Comparison of retrieved ozone profiles is complicated if the observations have different horizontal and vertical resolutions. Averaging kernels for both instruments have to be taken into account when different grids are used. Further, one must be careful to minimize interpolation errors when profiles are given on different pressure grids.

Apart from comparing ozone profiles, it might also be useful to take a measured ozone sonde profile and calculate the radiances at the top of the atmosphere. This makes it possible to validate separately the retrieval part of the algorithm, i.e. Optimal Estimation, and the radiative transfer part of the algorithm. Substantial calibration errors, either for the ozone sonde or the remote sensing instrument, can be found in this manner.

7.2.1.3 Tropospheric Ozone Column validation

The tropospheric ozone column product will provide gridded information on a daily or weekly basis. Correlative data should cover at least the entire troposphere and the lower stratosphere to establish a tropospheric column. In addition the correlative data should have the same temporal sampling as the tropospheric ozone column product.
Validation of tropospheric ozone columns can be performed using ground-based data like balloon sounding and satellite data from infrared sensors.

7.2.1.4 Key Parameters

- Total ozone column.
- Ozone vertical profiles from the surface to the upper stratosphere;
- Tropospheric ozone columns.

7.2.1.5 Spatial & Temporal Coverage Requirements

Global, covering all seasons.

7.2.1.6 Spatial & Temporal Sampling Requirements

Representativeness of observations (space and time) at the appropriate scales of approximately 10x10 km^2 for total ozone and 50x50km^2 for ozone profile and tropospheric ozone column.

7.2.1.7 Specific Short & Long-term Validation Aspects

TBD

7.2.2 Nitrogen dioxide (NO_2)

The nitrogen dioxide product consists of total and tropospheric columns. The latter are retrieved by separating the total column into the stratospheric and tropospheric components. Therefore, the tropospheric and stratospheric columns need validation as well as various input parameters needed in the retrievals.

The most important validation need for S5P NO_2 is for tropospheric NO_2 under polluted and clean conditions. Under polluted NO_2 conditions, column and profile information in the lower troposphere is essential for column density validation. The NO_2 data from previous instruments such as GOME, Sciamachy and OMI have been validated in several studies over the past years, based on satellite inter-comparisons (e.g. GOME-2, Sciamachy) as well as comparisons against ground-based (e.g. MAX-DOAS, Lidar) and in-situ (e.g. aircraft, balloon, surface) measurements. These validation activities have covered both tropospheric and stratospheric NO_2 data.

Despite these validation activities large uncertainties remain. These uncertainties are partly related to the quality of the independent NO_2 data used for the validation. Another important issue is representativeness of the often point-size ground-based and in-situ measurements relative to the spatially extended satellite ground pixels. In addition, the number of suitable validation data is very limited, making validation of the global data product difficult.

Use of satellite data for validation is useful as full global coverage and good statistics can be achieved directly comparing tropospheric columns. However, given the fact that also existing satellite data is not fully validated, these data sets can be only one component of the overall validation. When intercomparing satellite measurements, special care has to be taken to account for:

- differences in spatial resolutions, resulting in possible offsets between satellite observations,
- differences in overpass times,
- differences in a priori assumptions.

For the validation of the S5P NO_2 data shall include a better characterisation of the quality of the independent NO_2 data and any difference between these data sets and the S5P NO_2 data. These validation activities should make a distinction between stratospheric and tropospheric NO_2.

There is also a need for correlative data on quantities used in the retrievals, including surface albedo data to investigate the accuracy of the existing surface albedo climatologies and aerosol observations to better characterize the radiative transfer. Retrieval of S5P NO_2 also depends on cloud information, thus cloud properties must be validated carefully with correlative measurements.

Below plans for pre-launch (algorithm testing) and post-launch activities related to validation of the S5P NO_2 data product are listed. Post-launch activities include comparisons of geophysical data comparisons between S5P and correlative NO_2 data from a variety of sources.

For the ATBD reference, see [R11].

7.2.2.1 Algorithm testing and verification

Algorithm testing and verification is an important activity and provides confidence in the retrieval algorithms, including forward and inverse models, based on simulations, and comparisons between different techniques and software programs. Much of S5P's verification phase shall address this issue in a thorough way. This activity also includes reviews and updates of the S5P NO_2 ATBD.

7.2.2.2 Stratospheric NO_2 validation

For stratospheric NO_2 columns, correlative (column and profile) measurements are needed in regions that are representative for a complete zonal band, and hence need to be relatively unpolluted. Nevertheless, the measurements of stratospheric NO_2 concentrations taken from high-altitude ground stations, such as the Jungfraujoch station in Switzerland, are particularly valuable for validation.

Stratospheric NO_2 measurements near the Arctic vortex in late winter and early spring would be useful to better test the capability of a data assimilation scheme (and other stratosphere-troposphere separation schemes) in capturing the influence of stratospheric air masses low in NOx on stratospheric NO_2 at lower latitudes. Such excursions are known to occur and may lead to systematic errors in the separation. Independent measurements may provide important information on how to improve these issues.

7.2.2.3 Tropospheric NO_2 validation

For validation of tropospheric NO_2 data, correlative (column and profile) measurements are needed in the highly populated polluted regions at mid and low latitudes, and also in regions with natural sources of nitrogen oxides, e.g., from biomass burning, microbial soil activity and lightning. The validation data should extend to all relevant regions including Asia, Europe, America, and Africa, cover the full seasonal cycle and include background situations, regions with elevated pollution levels and pollution hot-spots.

Information on tropospheric NO_2 concentrations – with the NO_2 in the planetary boundary layer and/or in the free troposphere – comes from in-situ instruments (at the ground, in masts, or on low-flying balloons and aircrafts) and from remote-sensing instruments at the ground, on balloons or aircraft. The emerging suite of MAX-DOAS instruments is particularly valuable for validation of S5P measurements, but homogenisation and cross-calibration of these measurements should remain a priority for successful validation. In order to improve the coverage of spatial gradients and horizontal inhomogeneities in individual satellite pixels, moving platforms could play an important role.

An important issue when comparing independent NO_2 measurements with data derived from satellite-based instruments is the question of representativeness. We recommend a careful investigation into the spatial representativeness of any independent NO_2 measurement, in order to facilitate a meaningful comparison with the 7 km ×7 km sampling of TROPOMI.

Important for the validation from the TROPOMI measurements is a good understanding of the vertical profile of the tropospheric NO_2. The best source of information on vertical profiles of NO_2 is still from incidental aircraft campaigns. Alternatively, experimental NO_2 profiles from (tethered) balloon sondes, and measurement towers, can provide valuable information on the vertical distribution of NO_2.

Since tropospheric retrievals depend on the concept of the air-mass factor, which has to rely on a priori information, it is important to also validate the inputs and assumptions that go into the air-mass factor calculation. This concerns a number of parameters including surface reflectance, and cloud information such as cloud fraction and cloud pressure – that should be well characterised.

One critical issue, about which very little is known as yet, is the effect of the presence of aerosols on the NO_2 retrieval. Collocated information on the aerosol profile – e.g. coming from the S5P Aerosol Layer Height data product – could be useful for this.

7.2.2.4 Key Parameters

The most important validation need for S5P NO_2 is for tropospheric NO_2 under polluted and clean conditions.

7.2.2.5 Spatial & Temporal Coverage Requirements

Global - seasonal

7.2.2.6 Spatial & Temporal Sampling Requirements

Representativeness of observations (space and time); at the basic sampling scale, i.e. 7 x 7 km^2. Measurements should cover different pollution levels, different meteorological situations, different latitudes and the full seasonal cycle.

7.2.2.7 Specific Short & Long-term Validation Aspects

TBD

7.2.3 *Sulphur dioxide (SO_2)*

In order to validate the S5P SO_2 retrieval algorithm, comparisons with independent algorithms and measurements are required. Generally speaking, the validation of satellite SO_2 column products is a challenge for several reasons, on top of which is the representativeness of the correlative data when compared to the satellite retrievals. Intrinsically, the validation is never fully satisfactory as it makes a number of assumptions that probably will not hold under all conditions. Another reason comes from the wide range of SO_2 columns in the atmosphere that vary from about 1 DU level for anthropogenic SO_2 and low level volcanic degassing to 10-1000 DU for medium to extreme volcanic explosive eruptions.

The measurement of anthropogenic SO_2 is a difficult task because of the low column amount and reduced measurement sensitivity close to the surface. The SO_2 signal is generally overwhelmed by the competing O_3 absorption and the column accuracy is directly affected by the quality of the background correction applied. Among the many parameters of the SO_2 retrieval algorithm that affect the results, the SO_2 vertical profile shape is of utmost importance for any comparison with correlative data.

The measurement of volcanic SO_2 is facilitated by larger SO_2 columns than for anthropogenic SO_2. However, the total SO_2 column is strongly dependent on the height of the SO_2 plume, which is highly variable and very often unknown. For most volcanoes, there is generally no ground-based equipment to measure SO_2 during an appreciable eruption and even if it is the case, the data are generally very difficult to use for validation. For strong eruptions, volcanic plumes are transported over long-distances and can be measured by ground–based and aircraft devices but there is only a handful of datasets available and the number of coincidences is generally small.

For both anthropogenic and volcanic scenarios, inter-comparison of satellite SO_2 measurements generally improves the statistics but it poses a number of problems because the different satellite sensors available have different overpass time, swath, spatial resolution and measurement sensitivity to SO_2.

For the ATBD reference, see [R12].

7.2.3.1 Volcanic SO_2

Dedicated aircraft campaign flights can in principle measure volcanic SO_2 clouds, but rely on the occurrence of volcanic events. Their trajectory can be planned with relative ease to cross degassing volcanoes or sustained eruptive plumes. Localized SO_2 concentrations, for example due to (explosive) eruptions, may be carried away too quickly to be captured by aircraft or have diluted below the threshold limit for satellite detection before an aircraft can respond.

An important SO_2 database to be considered is provided by the CARIBIC project. Extensive measurements of many atmospheric constituents (including SO_2) are made during long distance flights on a regular basis and via automated scientific apparatus underneath the aircraft. Measurements of SO_2 during the eruptions of Mt. Kasatochi and Eyjafjallajökull have been compared to GOME-2 SO_2 data.

Several ground-based measurements of volcanic plumes exist that have been used for the validation of satellite data. GOME-2, Sciamachy, and OMI measurements of the 2008 Mt. Kasatochi plume over Europe have been compared with Brewer measurements in Uccle (Belgium) and Manchester (UK). Validation with ground-based spectrometers is challenging, because of the relatively fast displacement of the volcanic cloud with respect to the ground spectrometer and possible heterogeneity on scales smaller than to a TROPOMI pixel. Fast moving volcanic clouds therewith confirm the need for a static network of ground stations.

7.2.3.2 Anthropogenic SO_2

Comparisons of individual satellite SO_2 measurements and ground-based observations is challenging, due to satellite data scatter and cloud cover. Although the situation for S5P is expected to be better due to improved spatial resolution and S/N ratio, spatial and temporal averaging will be needed. In order to have reliable validation results, a suite of observations (e.g. ground based in-situ & remote sensing, airborne in-situ & remote sensing) that provide complementary information on the 3-dimensional distribution of tropospheric SO_2. In addition to measurements of SO_2, it is also essential to have information on the aerosol loading and aerosol optical properties. Such complete measurements can only be performed during measurement campaigns. In addition to these campaigns, long-term correlative data sets are needed to provide quality assessment throughout the mission.

7.2.3.3 Key Parameters

- Total column of SO_2;
- Profiles of SO_2 in the troposphere;
- Identification of the volcanic SO_2 plume height.
- Aerosol loading and optical properties in the UV.

7.2.3.4 Spatial & Temporal Coverage Requirements

- Volcanic SO_2: global covering degassing and eruptive volcanoes.
- Anthropogenic SO_2: regions for which the SO_2 concentrations exceeds the observational threshold.

7.2.3.5 Spatial & Temporal Sampling Requirements

- For volcanic plumes the rapid movement of the plumes makes that validations measurements should be made at the time over the S5P overpass.
- For anthropogenic SO_2 the spatial heterogeneity should be assessed.

7.2.3.6 Specific Short & Long-term Validation Aspects

TBD

7.2.4 Formaldehyde (HCHO)

To validate the S5P formaldehyde data products, comparisons with independent sources of HCHO measurements are required. This includes comparisons with ground-based measurements, aircraft observations and satellite data sets from independent sensors. As for other tropospheric data products, the validation of HCHO column measurements from TROPOMI is difficult and challenging. The effect of a priori vertical profiles, aerosols, clouds, albedo changes, and spatial gradients must be taken into account; however adequate correlative measurements are currently lacking to address these issues in a comprehensive and systematic manner.

For HCHO validation, not only information on the total (tropospheric) HCHO column is needed but also information on its vertical distribution, especially in the first three kilometres where the bulk of formaldehyde generally resides. In this altitude range, the a-priori vertical profile shapes have the largest systematic impact on the satellite column errors due to the strong decrease of the satellite UV measurement sensitivity near the surface.

The diversity of the NMVOC species, lifetimes and sources (biogenic, biomass burning or anthropogenic) ask for validation data in a large range of locations worldwide (tropical, temperate and boreal forests, urban and sub-urban areas). Continuous measurements are needed to obtain good statistics (as well for ground-based measurements as for satellite columns) and to capture the seasonal variations. Validation and assessment of consistency with historical satellite datasets require additional information on the HCHO diurnal variation, which depends on the precursor emissions and on the local chemical regime.

The main emphasis is on quality assessment of retrieved HCHO column amounts on a global scale and over long time periods. The validation exercise will establish whether HCHO data quality meets the requirements of geophysical research applications like long-term trend monitoring on the global scale, NMVOC source inversion, and research on the budget of tropospheric ozone. In addition, the validation will investigate the consistency between S5P HCHO data and HCHO data records from other satellites.

Although ground-based remote-sensing MAX-DOAS and FTIR instruments are naturally best suited for the validation of column measurements from space, in-situ instruments can also bring useful information. This type of instrument can only validate surface HCHO concentrations, and therefore additional information on the vertical profile (e.g. from regional modelling) is required to make the link with the satellite retrieved column. However, in-situ instruments have the advantage to be continuously operated for pollution monitoring in populated areas, allowing for extended and long term comparisons with satellite data.

The interpretation of comparisons between satellite HCHO measurements and MAX-DOAS/FTIR data is generally complicated by the noise of satellite data, interference by clouds and by the spatial gradients in HCHO that are generally sampled differently from the ground and from space. Although the situation for TROPOMI is expected to be improved owing to the high spatial resolution and S/N ratio of this instrument, spatial and temporal averaging will be needed to improve the statistics of comparison.

For adequate validation, the long-term monitoring should be complemented by dedicated campaigns such as the CINDI campaign (Cabauw, The Netherlands, Jun.-Jul. 2009). Ideally such campaigns should be organised in appropriate locations such as e.g. South-Eastern US, Alabama where biogenic NMVOCs and biogenic aerosols are emitted in large quantities during summer time.

For the ATBD reference, see [R13].

7.2.4.1 Satellite-satellite intercomparisons

Satellite-satellite intercomparisons of HCHO columns are generally more straightforward than validation using ground-based correlative measurements. Such comparisons are evaluated in a statistical sense focusing on global patterns and regional averages, seasonality, scatter of values and consistency between results and reported uncertainties.

When intercomparing satellite measurements, special care has to be drawn to:

- differences in spatial resolutions, resulting in possible offsets between satellite observations,
- differences in overpass times,
- differences in a priori assumptions.

Assessing the consistency between successive satellite sensors is essential to allow for scientific studies making use of the combination of several sensors. For example trends in NVMOC emissions could be successfully derived from GOME, Sciamachy, OMI and GOME-2 measurements It is anticipated that TROPOMI, the next GOME-2 instruments and the future Sentinel-4 and-5, will allow to extend these time series.

7.2.4.2 Key Parameters

- Total formaldehyde columns;
- Vertical profiles of formaldehyde during campaigns.

7.2.4.3 Spatial & Temporal Coverage Requirements

Sites operating correlative measurement should preferably be deployed at locations where significant NMVOC sources exist. These include:

- Tropical forests (Amazonian forest, Africa, Indonesia).
    - ➢ Largest HCHO columns worldwide.
    - ➢ Remote areas, difficult to access.
    - ➢ Biogenic and biomass burning emissions are mixed. A complete year is needed to discriminate the various effects on the HCHO retrieval.
    - ➢ Clouds tend to have more systematic effects in tropical regions.
    - ➢ Aircraft measurements over biomass burning.
    - ➢ HCHO and aerosols profiles measurements are needed, starting from the ground.
- Temperate forests (South-Eastern US, China, Eastern Europe).

  - In summer time, HCHO columns are dominated by biogenic emissions. Those locations are useful to validate particular a-priori assumptions such as model isoprene chemistry and OH oxidation scheme.
  - Measurements needed from April to September.
  - HCHO and aerosols profiles measurements are needed, starting from the ground.
- Urban and sub-urban areas (Asian cities, California, European cities)
  - Anthropogenic NMVOCs are more diverse, and have a weaker contribution to the total HCHO column than biogenic NMVOCs. This type of signal is therefore more difficult to validate.
  - HCHO and aerosols profiles measurements are needed, starting from the ground.
  - Continuous observations at mid-latitudes over a full year are needed, to improve statistics.

7.2.4.4 Spatial & Temporal Sampling Requirements

- Correlative observations should preferably be made at the time of the satellite overpass.
- In many cases the satellite data need to be averaged in space and/or time. Therefore correlative data should be representative for the entire spatial region and temporal period of the averaging.

7.2.4.5 Specific Short & Long-term Validation Aspects

TBD

7.2.5 Carbon monoxide (CO)

The validation of the CO product will primarily be based on systematic comparisons with ground-based total column measurements. There are currently two important networks that perform total column CO measurements: TCCON and IRWG/NDACC. The Total Carbon Column Observing Network (TCCON, https://tccon-wiki.caltech.edu) is a network of ground-based Fourier Transform Spectrometers recording direct solar spectra in the near-infrared spectral region in the spectral range between 0.7 and 2.5 μm. The Infrared Working Group (IRWG, http://www.acd.ucar.edu/irwg/) represents a similar network of infrared solar Fourier-transform spectrometers that is part of the Network for the Detection of Atmospheric Composition Change (NDACC). It is a multi-national collection of over twenty high-resolution spectrometers that regularly record the atmospheric absorption spectrum from sites distributed from pole to pole. It should be noted that in terms of geo-location the NDACC and TCCON network have a large overlap. Furthermore most of the NDACC and TCCON sites are situated in remote locations and in Europe and North America.

Vertical profiles of CO will allow for detailed validation of the product, taking into account the averaging kernel. Vertical profiles can be measured from aircrafts, as for example done during ascents and descents on IAGOS MOZAIC flights. Another technique to measure the profile of CO is the AirCore and has the potential to provide a ground-truth standard for comparison with total column measurements from either ground-based Fourier Transfer Spectrometers or satellites.

Ground based in-situ measurements of CO are routinely made in air quality networks. Although such measurements cannot provide information on the total column, they do allow assessments of the horizontal distribution on the sub-TROPOMI pixel-scale.

For the ATBD reference, see [R14].

7.2.5.1 Satellite intercomparison

MOPITT (Measurements of Pollution in the Troposphere) is a payload scientific instrument launched into orbit by NASA on board the Terra satellite in 1999. It is designed to monitor changes in pollution patterns. MOPITT measurements yield atmospheric profiles of CO volume mixing ratio and CO total column values using near-infrared radiation at 2.3 μm and thermal infrared radiation at 4.7 μm. For the validation of the S5P CO data product, an inter-comparison with the MOPITT near-infrared data product will be very useful and has to be seen complementary to the validation using ground based measurements. However, it is not clear if the MOPITT instrument will be still operational when the S5P mission will be launched.

CO is also measured from FTIR satellite instrument like IASI, TES and AIRS, which offers another opportunity for comparisons. However, the measurements in the FTIR have significantly lower sensitivity to the lower troposphere, as compared to the SWIR measurements of TROPOMI which should be considered in the intercomparisons.

7.2.5.2 Key Parameters

CO total column and CO vertical profile.

7.2.5.3 Spatial & Temporal Coverage Requirements

Global over land; for all seasons. It is essential to validate the CO product for a variety of atmospheric conditions, like polluted and clean conditions, humid and dry air samples and bright and dark surface types. Also different solar and viewing geometries of the observation have to be considered. Validation cases should be performed up to cloud fractions of 0.5.

7.2.5.4 Spatial & Temporal Sampling Requirements

TBD

7.2.5.5 Specific Short & Long-term Validation Aspects

TBD

7.2.6 Methane (CH_4)

Due to the long lifetime of methane in the atmosphere the spatial and temporal variability of the total column is small. This leads to high accuracy requirements for the S5P methane product and thus to even tighter requirements to correlative data sets. An important data set for the validation will be the TCCON network, which has become the standard for validating satellite based column measurements of CO_2 and CH_4 TCCON XCH_4 measurements have been calibrated and validated against the WMO-standard of in-situ measurements using dedicated aircraft campaigns of XCH_4 profiles and their resulting accuracy have been estimated to 0.4% (2σ value). An important limitation of the TCCON network for validation of S5P methane retrievals is limited coverage in areas with high surface albedo and in the Tropics. Alternatives to the TCCON network should have a comparable accuracy.

In situ measurements of the full vertical CH_4 profile will be extremely useful as they allow the column averaging kernel to be applied and hence the retrieved XCH_4 from S5P can be compared with truly the same quantities. TCCON only delivers the column integrated values and hence do not allow the averaging kernel to be applied, which leads to a remaining uncertainty in the comparison. Vertical profiles can be obtained by aircrafts as is done for calibrating the TCCON network, but they do not sample the full total column. In this respect a very interesting new development is provided by the AirCore initiative.

For the ATBD reference, see [R15].

7.2.6.1 Satellite Intercomparison

GOSAT has been launched in 2009 and provides column integrated XCH_4 with sensitivity to the ground making use of the 1.6 micron channel. GOSAT can make use of both the proxy method as well as a Full Physics method such as developed for S5P. The RemoTeC algorithm, on which the S5P algorithm is based, is continuously being applied to the global GOSAT Level 1 data set. Therefore, comparisons with GOSAT will be very useful. However, it is not clear if GOSAT is still active when the S5P instrument will be launched. The GOSAT-2 instrument is planned for launch in 2018 so may be used for S5P validation/comparison purposes later in the mission. Likely, GOSAT-2 will also have a spectral band around 2300 nm, like S5P, and will hence be even more interesting to validate/compare to S5P.

7.2.6.2 Key Parameters

- Total column CH_4;
- Vertical profiles of CH_4.

7.2.6.3 Spatial & Temporal Coverage Requirements

Global over land, covering the complete range of surface albedo’s including low and high albedos, and covering all seasons.

7.2.6.4 Spatial & Temporal Sampling Requirements

TBD

7.2.6.5 Specific Short & Long-term Validation Aspects

TBD

7.2.7 Aerosols

The S5P L2 aerosol products focus on two parameters: the Aerosol Absorbing Index (AAI) and the Aerosol Layer Height (ALH). In addition the ALH algorithm also provides an effective aerosol optical thickness, derived at approximately 750 nm using a fixed aerosol phase function and single scattering albedo. Whereas the AAI is a product that has a long heritage from the TOMS, GOME, Sciamachy, OMI and OMPS instrument, the ALH is recent development.

The AAI is a special product because it is not a geophysical quantity. Therefore, there is no direct way of validating the AAI using correlative data. The AAI is very sensitive to the radiometric calibration in the spectral range between 340 and 400 nm. As such, validation of the AAI has been performed traditionally as part of the Level 1B. Given the importance of the radiometric calibration for long-term monitoring, an important activity of the AAI validation is the intercomparison between different instruments.

A large-scale global validation of the Aerosol Layer Height product is essential to understand the quality and performance of the sensor and algorithm. Substantial validation will also increase the product’s usability. The first focus of the ALH is on elevated aerosol plumes of moderate to high optical thickness, e.g. biomass burning, desert, volcanic and pollution plumes. The ALH can only be retrieved for cloud free scenes. For the validation it is essential to have observations of the aerosol extinction or backscatter profile, as for example can be measured using LIDAR systems. The correlative measurements should be preferably made at the time of the S5P overpass, and representative for at least one ground pixel ($7x7km^2$). In addition to the profile information, characterisation of the aerosol optical properties (aerosol optical thickness, phase function, single scattering albedo) is valuable to understand the impact of a-priori information on the retrieval.

As the ALH algorithm is a new data product, it is essential to collect a set of cases, which are fully characterised in terms of aerosol profile and aerosol optical properties, as well as surface albedo. These case studies could be the focus of a campaign. In addition to these case studies, a global validation covering all season is required.

Intercomparison with active satellite sensors, such as CALIOP on board Cloud-Aerosol Lidar and Infrared Pathfinder Satellite Observation (CALIPSO, in orbit since 2006) and the atmospheric lidar on ADM-Aeolus (expected launch date 2015) but also lidar as part of the Earth Clouds, Aerosols and Radiation Explorer (EarthCARE) mission (expected launch date end of 2016), should be part of the global validations.

A number of other passive satellite retrievals of aerosol height can be used for an intercomparison with ALH. We mention aerosol plume height retrievals over sea from the ratio of reflectances in MERIS channels at the O_2 A-band, stereo height retrievals for smoke plumes with clearly discernable sources from the Multi-Angle Imaging

Spectroradiometer (MISR), and dust height retrievals from the IASI hyperspectral thermal infrared measurements.

For an internal consistency check of the ALH algorithm, data sets from different satellite platforms can be compared. The ALH algorithm will be applied to GOME-2 and Sciamachy in the pre-launch phase as part of TROPOMI algorithm development. In addition, the aerosol profile retrieval concept for Sentinel-4 prepared by KNMI continues and builds upon the TROPOMI ALH algorithm. The Sentinel-4 / Ultraviolet Visible Near-Infrared (UVN) instrument on board the geostationary Meteosat Third Generation - Sounder (MTG-S) satellite is planned for launch in 2019.

For the ATBD reference, see [R16].

7.2.7.1 Key Parameters

- AAI validation focuses on the calibration of the radiances in the UV part of the spectrum 340-400 nm.
- For validation of the ALH the key parameter is the vertical aerosol profile.

7.2.7.2 Spatial & Temporal Coverage Requirements

Global, covering all seasons

7.2.7.3 Spatial & Temporal Sampling Requirements

ALH validation should focus on cloud-free regions with moderate to high aerosol optical thickness. Correlative data should be representative for at least one TROPOMI pixel (7x7 km^2).

7.2.7.4 Specific Short & Long-term Validation Aspects

TBD

7.2.8 Clouds

There are two cloud products relevant to S5P/TROPOMI:

- The S5P products that provides cloud fraction, optical thickness (albedo) and cloud height (pressure) from the TROPOMI measurements;
- Selected cloud information from the VIIRS instrument on board of the US S-NPP mission, aggregated on the TROPOMI footprints.

7.2.8.1 Internal Cloud Product

Because of the spatial-temporal heterogeneity of clouds, validation of cloud properties can be best done using satellite intercomparisons. For TROPOMI the best opportunity is with the US S-NPP mission that is planned to fly in loose formation with S5P, however also several of the NASA A-Train missions with cloud sensors will have frequent overlaps with the TROPOMI swath.

The VIIRS instrument has a Level 2 cloud product that covers amongst others the cloud fraction, cloud optical thickness (albedo) as well as the cloud top height (pressure). The OCRA/ROCINN algorithms working in the DOAS- and GODFIT-ozone GDP4.0 and GDP 5.0 environment were validated in a similar way by comparing GOME cloud parameters to values derived from collocated measurements from the ATSR-2 instrument (alongside GOME on the ERS-2 platform). The same applies to comparison performed between cloud parametres from Sciamachy and AATSR on the ENVISAT platform and between GOME-2 and AVHRR on the MetOp platforms. In addition to the imagers, the TROPOMI cloud products can also be compared to the OMI clouds products, provided that there is sufficient overlap between OMI and TROPOMI.

In addition to satellite intercomparisons, also ground-based as well as airborne measurement maybe useful. Especially radars can provide unique information on the vertical structure of clouds.

For the ATBD reference, see [R17].

7.2.8.1.1 Key Parameters

- Cloud fraction;
- Cloud optical thickness (albedo);
- Cloud height (pressure).

7.2.8.1.2 Spatial & Temporal Coverage Requirements

Global and covering all seasons. All cloud types should be adequately sampled. Especially challenging regions are above snow and ice.

7.2.8.1.3 Spatial & Temporal Sampling Requirements

Given the spatial-temporal heterogeneity of clouds, close time coincidences are essential.

7.2.8.1.4 Specific Short & Long-term Validation Aspects

Apart from the comparison with correlative observations, also algorithm verification will provide important information on the quality of the S5P cloud products. The verification activities, which started already before launch with the comparisons of the OCRA/ROCINN and the FRESCO algorithm, are expected to continue after launch.

Long-term validation should focus on contributing to the creation of a cloud ECVs from O_2 A-band measurements from GOME-type sensors.

7.2.8.2 S-NPP Cloud-Product for TROPOMI

The S-NPP/S5P cloud product is simply a resampling of the S-NPP cloud product and the S-NPP L1B product for selected spectral bands on the TROPOMI ground pixels. As such the independent validation of this product relies primarily on the validation of the VIIRS data product. Note that cloud fractions in the S-NPP-S5P product represents the geometric fraction of cloudy scenes at VIIRS spatial resolution, whereas the TROPOMI cloud fraction is an effective quantity intended to represent the effect of cloud on TROPOMI measurements. Although comparisons between these two products should not be expected to agree perfectly, it is nevertheless considered useful to perform systematic inter-comparisons of the fractions derived from the two techniques. E.g. changes in the level of agreement over time would indicate changes in the performance of one or other product.

For the ATBD reference, see [R18].

7.2.8.2.1 Key Parameters

- Cloud fraction;
- Cloud albedo;
- Vertical extinction profile.

7.2.8.2.2 Spatial & Temporal Coverage Requirements

Global and covering all seasons. All cloud types should be adequately sampled. Especially challenging regions are above snow and ice.

7.2.8.2.3 Spatial & Temporal Sampling Requirements

Given the spatial-temporal heterogeneity of clouds, close time coincidences are essential.

7.2.8.2.4 Specific Short & Long-term Validation Aspects

TBD

7.2.9 Surface UV Product

The S5P UV Product includes a suite of surface UV irradiances. The irradiances are given both at specific wavelengths and as weighted by biological action spectra such as the erythemal weighting function for sunburn of human skin. Moreover, the irradiances are provided corresponding to the satellite overpass time, local noon, and as daily doses. The S5P UV Product further includes the cloud optical thickness needed to calculate the surface UV irradiances.

The S5P UV Product is essentially based on radiative transfer calculations, given inputs defining the total ozone column (from S5P), the atmospheric aerosol content (from a climatology), the cloud optical thickness (from S5P UV algorithm or possibly elsewhere), and the surface albedo (from a climatology). The uncertainty of the UV Product largely arises from uncertainties in the aforementioned input parameters.

Therefore, it is important that validation studies include both (1) large scale, global or near-global analyses aiming to assess the overall performance of the S5P UV Product and (2) detailed studies aiming to understand the role of individual input parameters such as clouds or aerosols. In particular in the case of more detailed validation studies, it is important to consider the representativeness of both the S5P UV products and the reference data so that, for example, ground-based UV irradiances are matched in time with the satellite overpass. For assessing the overall performance, also validation against other satellite UV products may be useful.

The variation in cloud optical properties is a main driver of variations in the surface UV irradiance. Therefore, validation of the cloud optical thickness is of particular interest. Other satellite products such as VIIRS or MODIS can be used for comparison, as well as ground-based remotely sensed cloud optical thicknesses.

7.2.9.1 Key Parameters

- Ground-based, well-maintained and characterized UV irradiance measurements
- Other satellite UV products
- Cloud optical thicknesses from independent sources such as other satellite instruments or ground-based remote sensing
- Aerosols
- Surface albedo

7.2.9.2 Spatial & Temporal Coverage Requirements

- Global coverage would be ideal, important to span various climatic conditions
- Temporal coverage/sampling that enables a representative comparison between the S5P UV Product and the reference

7.2.9.3 Spatial & Temporal Sampling Requirements

- Representativeness and colocation in space and time are important

7.2.9.4 Specific Short & Long-term Validation Aspects

TBD

7.3 Optional Products

In addition to mandatory products also S5P optional products have been identified that have a potential to become operational at a later stage of the mission (see Table 3). However, in the context of this document addressing geophysical validation requirements, the focus is on the mandatory products for which requirement specifications have been provided above. This will not been done for optional products except for the Surface UV products (see Section 7.2.9).

Optional products include

- Water vapour - H_2O
- Glyoxal – CHOCHO
- Bromine monoxide - BrO
- Chlorine dioxide - OClO
- Deuterated water/water ratio - HDO/H_2O
- Surface UV[2]
- Aerosol Optical Depth AOD

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[2] The Surface UV product might get upgraded to a ‘mandatory product’.

However, proposals for validation of optional products from S5P will not per se be discarded simply because they are not belonging to the present list of mandatory S5P products. On a case-by-case basis, it shall be decided whether the proposed validation activities are feasible, useful and relevant for the S5P mission.

8 VALIDATION METHODS & TOOLS

8.1 Correlative Measurements

8.1.1 Airborne campaigns

During dedicated campaigns, aircraft and/or balloon measurements (at specific sites and seasons) involving combinations or `clusters' of large multi-instrument payloads shall be deployed.

The advantage of the airborne campaigns is the possibility to bridge the spatial scales stepwise, from ground via airborne to spaceborne measurements. Airborne in-situ measurements can deliver vertical profile information of one or more species with a high vertical resolution.

In such a way it is possible to characterise the temporal and spatial scale of the uncertainties in greater detail. In addition the representativeness of observations can also be addressed. However, it is recommended to actively participate in already scheduled activities in order to maximize gain.

8.1.2 Ground Based Campaigns

The target of ground-based validation campaigns is to provide a reference assessment for the overall S5P product generation chain exploiting a wide range of collocated reference instruments. This includes a detailed assessment of the operational processing steps, as well as for the overall product content. It shall specifically address critical elements, e.g., sub-satellite resolution cloud contamination or horizontal gradients, which cannot be addressed by single instrument observations. Both scientific instrumentation run in research modes as well as instruments intended for long-term monitoring shall participate, providing an opportunity for inter-comparison, and potentially inter-calibration of the ground-based instruments. Whenever feasible, ground based and airborne campaigns (see Section 8.1.1) shall be collocated or at least be planned in coordination to achieve the highest possible synergies from the investment.

The campaigns need to be implemented according to a campaign plan. The campaign plan shall provide a traceability from the validation objectives as defined by the product responsibles, to the measurement and instrumentation requirements the functional campaign baseline specifying the campaign location and time, specific instrumentation, their detailed set-up of and measurement timelines. A preliminary list of instruments can be extracted from the Validation Requirements detailed in Section 7 and includes: MAX-

DOAS, Brewer, FTIR, Lidar as well as in-situ measurement from balloons, AirCore and ground based measurements. Several competing aspects regarding place and time have to be considered in the planning such as availability of satellite data, status of calibration and Level 2 processors, campaign site availability, meteorological (including "chemical" weather) conditions. Due to the high organisational effort and the costs of ground-based campaigns, their detailed planning with respect to the S5P mission is critical importance and needs to be addressed in the campaign plan.

The scope and number of the ground-based campaigns depend on the availability of resources and the need based on the S5P mission evolution. Currently the objective is to have one major ground-based campaign at the beginning of the mission. In the course of the mission, additional validation activities might be added to existing field campaigns which are organised in a non S5P frame or smaller dedicated campaigns, e.g., for the intercomparison of key operational validation systems.

8.1.3 Existing Networks

A number of projects and initiatives are, or will be, providing data from measurement networks for the validation of S5P products. It is essential to differentiate between physical networks, activities coordinating instrument networks, thematic data centres archiving and providing validation data from measurement station, and projects focussing on specific aspects of measurement networks.

The international Network for the Detection of Atmospheric Composition Change (NDACC) [R-I5] is composed of more than 70 high-quality, remote-sensing research stations for observing and understanding the physical and chemical state of the stratosphere and upper troposphere and for assessing the impact of stratosphere changes on the underlying troposphere and on global climate. It is a major contributor to the worldwide atmospheric research effort, consists of a set of globally distributed research stations providing consistent, standardized, long-term measurements of atmospheric trace gases, particles, spectral UV radiation reaching the Earth's surface, and physical parameters, in particular focussing on detecting changes and trends in atmospheric composition and understanding their impact on the stratosphere and troposphere. The NDAAC observational capabilities include lidars, microwave radiometers, UV/Vis spectrometers, FTIRs, Dobson and Brewer instruments, sondes, as well as UV spectroradiometers.

TCCON [R-I6] is a network of ground-based Fourier Transform Spectrometers that record direct solar spectra in the near-infrared. From these spectra, accurate and precise column-averaged abundances of atmospheric constituents including CO_2, CH_4, N_2O, HF, CO, H_2O, and HDO, are retrieved. TCCON currently consists of around 20 different operational sites spread globally.

The AErosol RObotic NETwork (AERONET) [R-I7] program is a federation of ground-based remote sensing aerosol networks. The program provides a long-term, continuous and readily accessible public domain database of aerosol optical, mircrophysical and radiative properties for aerosol research and characterization, validation of satellite retrievals, and synergism with other databases. The network imposes standardization of instruments (spectral sun photometers), calibration, processing and distribution. Data of spectral aerosol optical Depth (AOD), inversion products, and precipitable water in diverse aerosol regimes are provided.

Other networks include the WMO-GAW coordinated global network of ozone sondes, with the SHADOZ [http://croc.gsfc.nasa.gov/shadoz/] [R-I8] project providing around 12 ozone sonde sites in low and low-southern latitude. In addition to the sondes, Brewer and Dobson instruments are providing data to the World Ozone and Ultraviolet Radiation Data Centre (WOUDC) [R-I9].

There are further a number of projects aiming at the operationalization, harmonisation and intercalibration of existing measurement systems. For example, the NORS (Demonstration Network Of ground-based Remote Sensing Observations in support of the Copernicus Atmospheric Service) [R-I10] Project aims at demonstrating the value of ground-based remote sensing data from the NDACC for the operational quality assessment and improvement of the Copernicus Atmospheric Service products. The EUropean BREWer NETwork (EUBREWNET) [R-I11] initiative aims at coordinating Brewer Spectrophotometer measurements of ozone, spectral UV and aerosol optical depth (AOD) in the UV within Europe, and unite the ozone, UV and AOD communities, through a formally managed European Brewer Network capable of delivering a consistent, spatially homogeneous European data resource. In order maintain and secure the data quality within a network dedicated intercalibration activities are necessary, like the ESA CEOS Intercalibration project. New instrument networks may emerge in the future. There are, for example, efforts to establish a small network of Pandora mini-spectrometer systems in Europe or ideas for low-cost FTIR instruments that can complement the TCCON measurement systems.

The national environmental agencies are operating instrument networks for the monitoring of local or regional air quality, which also include species covered by S5P. However, the measurements are usually taken at street level in urban locations, which complicates their usage for the validation of satellite retrievals because they are usually not representative for larger areas equivalent to satellite footprints.

8.1.4 Satellite Intercomparisons

The intercomparison between similar products from different satellite missions can provide important information for the assessment single instrument's Level 1b and Level 2 quality. The comparison, however, needs to carefully assess the differences between the satellites and their retrievals, such as difference in local time, horizontal representativeness, vertical sensitivity, a-priory information, cross-sections, etc. As compared to the stratospheric product comparisons this has to be considered in much more detail due to the spatial and temporal variability of air-quality products.

There are several satellite missions that are expected to be operational during the S5P operational lifetime (2016-2022) that can contribute to satellite intercomparisons, such as GOME-2 on MetOp, OMPS on S-NPP and OCO-2. At a later stage, the geostationary air-quality systems GEMS, GMAP-ASIA, Sentinel-4 and TEMPO are expected to be available, as well as the planned GOSAT follow-up mission. Towards the end of the S5P mission a significant overlap with Sentinel-5 is expected. The currently operational missions that can provide correlative for S5P data are all coming to their design end-of-life, which does not exclude that some are still providing data at the time of the S5P launch. These systems include in particular OMI on Aura, GOSAT and MOPITT on Terra. An overview of the past, current and future missions are for example provided by the NDACC Satellite Working Group [R-I12].

8.2 Impact Experiments

To investigate the impact of various types of data on numerical forecasts, observing system experiments are performed using assimilation algorithms. This might include e.g. data denial experiments.

Observational data from S5P might provide valuable insights into the impact of, for example, aerosols on atmospheric chemistry. Aerosols can impact atmospheric chemistry in several ways. They can affect the actinic flux and thus alter photolysis rates. In addition, through radiative forcing effects, they can change the regional temperature and cloud fields, which in turn may perturb the photochemical processes. These impacts of aerosols on tropospheric chemistry have so far remained poorly characterized.

Therefore, such activities are also expected to be carried out as part of the S5P validation activities.

9 CONCLUSIONS

The above requirements for geophysical validation describe the Level-2 products and their respective accuracies. These numbers shall provide guidelines to the potential proposers for the validation methods to be identified but, on purpose, the document does not prescribe any method. Potential methods shall be identified by the proposers in their responses to the AO Call.

This document shall also serve as a reference for the reviewers of the AO proposals as they should screen the proposals submitted against these geophysical requirements. Furthermore, the document shall help identifying gaps in the validation of the S5P mission which would potentially need to be addressed in updates of the Cal/Val Implementation Plan [A1].