

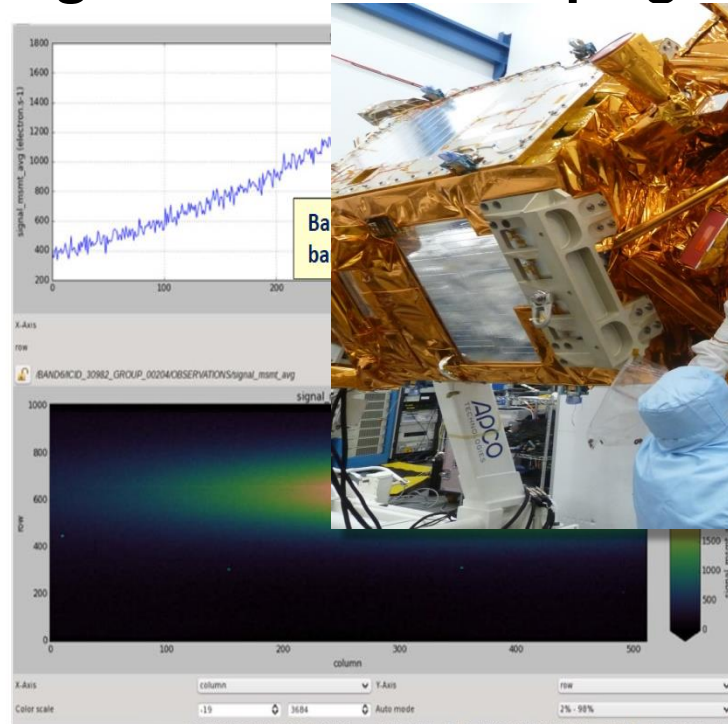


Sentinel-5 Precursor Mission and Cal/Val lessons learned

C. Zehner (ESA) & J.-C. Lambert (BIRA-IASB)

Importance of the pre-flight calibration campaign!

- unexpected response observed in pre-launch calibration measurements;
-> NIR channel (661 – 786 nm)
- origin & magnitude of effect initially unclear
- analyses of spectral filters & light sources revealed signals originated by emissions at wavelengths > 800 nm



Pre-flight calibration problem (straylight in the NIR) solved during time period of the launch delay – Dec. 16/Jan. 17 at Airbus D&S / UK

AC-VC-16 Meeting Slide 2

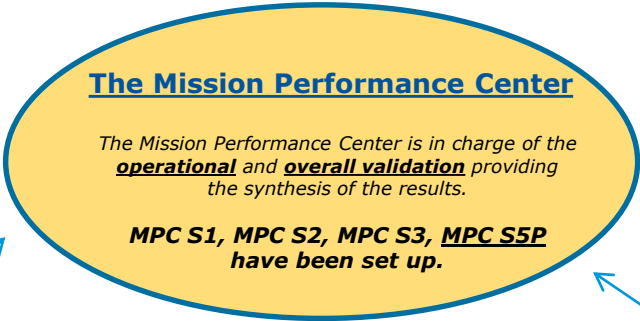
CalVal WORKSHOP # 2 | ESTEC 15 & 16 February, 2018 | Slide 5

Importance of the pre-flight calibration campaign!

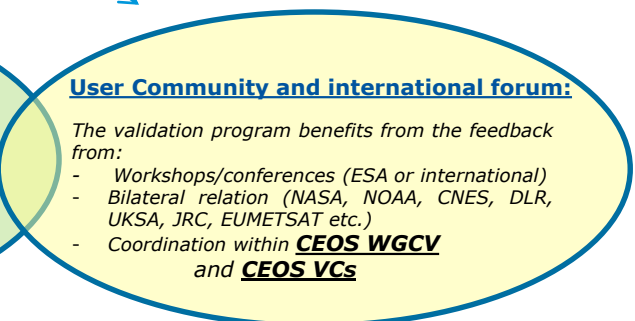
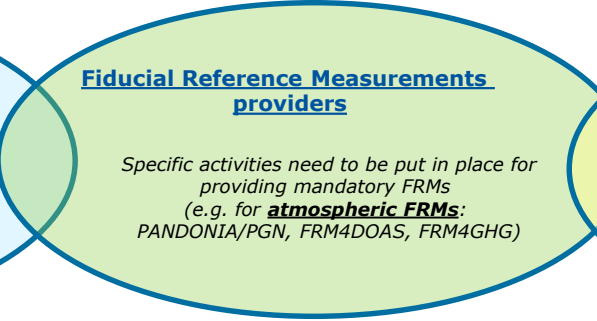
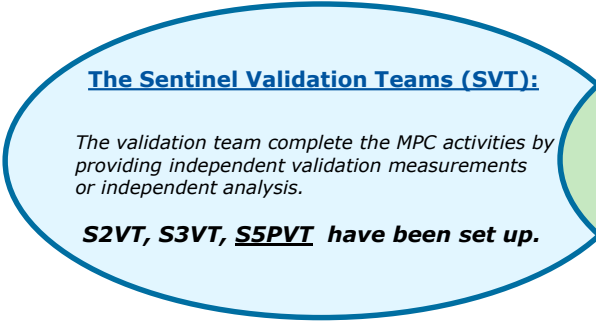
All Sentinel-5 Precursor Products have been delivered so far to the public except the Ozone Profile – reason: problems during the pre-flight calibration campaign causing wrong calibration in the UV wavelength range for sun irradiance measurements

Solution: ‘adjustment’ of Sentinel-5P irradiance measurement to Suomi-NPP OMPS irradiance measurements

SENTINEL VALIDATION TEAM : The validation team complete the MPC activities by providing independent validation measurements or independent analysis. The team members are selected through an open call process. The intention of this call is to create scientific validation teams to provide structured coordination of international activities that contribute to Sentinel validation across the entire mission (i.e. Phase E1 and E2).



The information is then discussed, further processed in the **Quality Working Groups** which provide synthetic results to the **Mission Managers**, used for improving the products quality and the products knowledge.



MPC Routine Operations Validation



To the Automated Validation Server

VALIDATION FACILITY

SENTINEL 5P MISSION PERFORMANCE CENTER



Results and resources by product

Most recent contributions

- Validation against SHADOZ ozonesonde data confirms that the TROPOMISp OFFL tropospheric O3 (L2_O3_TCL) data product meets mission requirements. This web article summarizes the results of the validation of the first year of SP OFFL tropospheric ozone column data products (v01.01.05, v01.01.06 and v01.01.07) against co-
- First comparison results for the S5P CH4 product based on correlative reference measurements acquired by FTIR instruments contributing to NDACC and TCCON networks.
- First validation results for Sentinel-5P NO2 column data. This report describes initial validation results for Sentinel-5P TROPOMI L2_NO2 tropospheric column, stratospheric
- First validation against NDACC and VIZOCC ground-based data confirms that the TROPOMI S5P NRTI total O3 (L2_O3) product meets mission requirements. Initial Sentinel-5P
- Preliminary comparison of TROPOMI S5P H2O CLOUD O3 cloud top height and CFB cloud height against ground-based CLOUDNET data. From the Sentinel-5P TROPOMI L2_CLOUD
- First comparison results for the S5P CO product based on correlative reference measurements acquired by FTIR instruments contributing to NDACC and TCCON networks.

ROCVR Reports

- Quarterly Validation Report of the Sentinel-5 Precursor
- Quarterly Validation Report of the Sentinel-5 Precursor
- Quarterly Validation Report of the Sentinel-5 Precursor
- Quarterly Validation Report of the Sentinel-5 Precursor

Quarterly Routine Validation Report

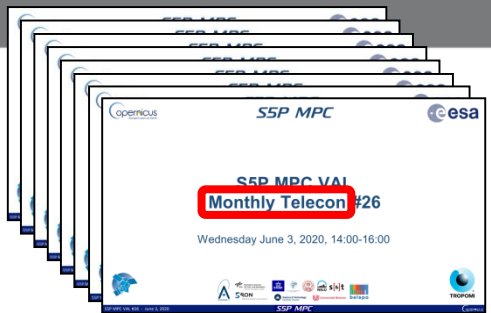
Validation Web Articles produced jointly by S5P MPC and S5PVT AO projects

TROPOMI
TROPOspheric Monitoring Instrument



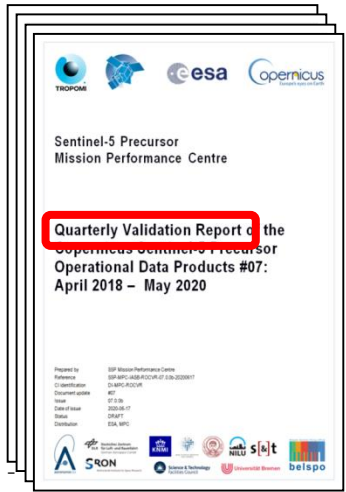


S5P MPC Quality Information Output



S5P MPC VAL
Monthly Telecon #26

Wednesday June 3, 2020, 14:00-16:00



Quarterly Validation Report of the Copernicus Sentinel-5 Precursor Operational Data Products #07: April 2018 – May 2020

Representative Quality Indicators

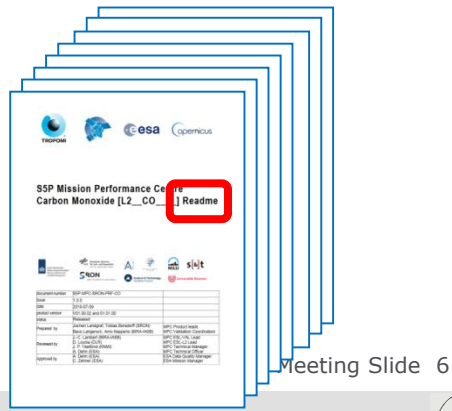
Based on the validation results reported in this document, representative values of key quality indicators (bias and spread) have been derived for the following S5P operational data products:

Product ID	Stream	Product	Bias	Dispersion	Special features
L2_O3	NRTI	O ₃ column	0.8%	2.5%	Larger dispersion over snowice due to coarse surface albedo climatology
	OFFL	O ₃ column	0.3%	2%	
L2_O3_TCL	OFFL (CCD)	O ₃ tropospheric column	+14%	23%	Positive bias over biomass burning. Geographical imprints of sampling-related biases.
L2_NO2	NRTI	NO ₂ troposphere NO ₂ stratosphere NO ₂ total	-22% -9% 0±50%	3.6 Pmol/cm ² 0.4 Pmol/cm ² -	Total NO ₂ bias depending on total column: pristine areas to slight pollution overestimated, high pollution underestimated.
	OFFL RPRO	NO ₂ troposphere NO ₂ stratosphere NO ₂ total	-23% -9% 0±50%	3.6 Pmol/cm ² 0.3 Pmol/cm ² -	
L2_HCHO	NRTI	HCHO low	+26%	7 Pmol/cm ²	Positive bias over clean areas (<2 Pmol/cm ²), negative bias over large emissions (> 8 Pmol/cm ²).
	OFFL RPRO	HCHO high	-31%	13 Pmol/cm ²	
L2_SO2	NRTI	SO ₂ column	0.2 DU	0.2 DU	Lack of validation sites in areas with high SO ₂ .
	OFFL	SO ₂ column	0.2 DU	0.2 DU	
L2_CO	NRTI	CO column	6.5%	5%	Along orbit stripes. High pollution underestimated. 5% SZA dependence of bias. Outliers in SAA and other sporadic locations not filtered by qa_value. Since July 2019 NRTI similar as OFFL.
	OFFL	CO column	6.5%	5%	
L2_CH4	OFFL	CH4 column	-0.27%	0.6%	Along orbit stripes. Underestimation at low albedo. Remaining outliers with qa_value>0.5. 1-4% seasonal and SZA dependence of bias.
L2_CLOUD	NRTI	CAL CTH CRB CH CAL COT	-20% -30% +7.9 [-]	2 km 1 km -	Bias towards the a priori cloud height up to and including 01.01.07. Snowice degrades retrievals. Occurrence of C[CTH] equal to surface height at low cloud fraction. Across track CTH and CF pattern. North-South cloud albedo pattern. COT positive bias vs VIIRS.
	OFFL	CAL CTH CRB CH CAL COT	-20% -30% +7.9 [-]	2 km 1 km -	
	NRTI	aerosol index	-1.1 AI unit	0.1 AI unit	
L2_AER_AI	OFFL	aerosol index	-1.1 AI unit	0.1 AI unit	Negative bias exceeding 1 AI unit after March 2019, attributed to irradiance data degradation.
	OFFL	aerosol layer height	50 hPa	100 hPa	Over ocean only. Larger bias and dispersion expected over land.

Table 2 – Representative quality indicators (bias, dispersion and special features) as estimated from the validation studies of the S5P TROPOMI operational data products identified in the Table 1. The processor version number is not mentioned as the estimates are representative for all versions available publicly. CTH: cloud-top-height; CH: cloud height; COT: cloud optical thickness.



Validation Web Article: Dry air column averaged methane



Readme

ESA UNCLASSIFIED



S5P MPC



European Space Agency



ESA FRM programme + WMO GAW contributing networks

S5P ID	S5P Data Product	Fiducial / Validation Reference Measurements
L2_O3	O ₃ total column	Brewer , Dobson , ZSL-DOAS , PGN/Pandonia
L2_O3_PR	O ₃ profile (incl. troposphere)	ozonesonde , stratospheric DIAL , tropospheric DIAL
L2_O3_TCL	O ₃ tropospheric column	ozonesonde
L2_NO2	NO ₂ stratospheric column	ZSL-DOAS
	NO ₂ tropospheric column	MAX-DOAS
	NO ₂ total column	PGN/Pandonia
L2_SO2	SO ₂ total column	MAX-DOAS , PGN/Pandonia
L2_HCHO	HCHO total column	MAX-DOAS , NDACC FTIR , PGN/Pandonia
L2_CO	CO total column	NDACC FTIR (MIR) , TCCON FTIR (NIR)
L2_CH4	CH ₄ total column	NDACC FTIR (MIR) , TCCON FTIR (NIR)
L2_CLOUD	Cloud Fraction	<i>not available (satellite-to-satellite only)</i>
	Cloud Height (pressure)	Cloudnet lidar/radar , ARM
	Cloud Optical Thickness	<i>not available (satellite-to-satellite only)</i>
L2_AER	UV Aerosol Absorbing Index	<i>not available (satellite-to-satellite only)</i>
	Aerosol Layer Height	EARLINET aerosol lidar , EUMETNET/ALC ceilometer

Colour code: **automated, full stream** automated, partial stream manual in development



Generic validation chain, state-of-the-art co-locators, harmonised terminology and comparison metrics... in permanent evolution

Chapter 10
Comparative merging of Vapour Observations: Multi-dimensional perspective on data sampling issues

Atmospheric Measurement Techniques

Round-robin methodology and metrology of model data

14 limb and occu

Harmonization and comparison State observation methods, of

Terms and definitions applicable to the quality assurance of Essential Climate Variable data records

Abstract. Comparisons are presented for a large number of data sets from a number of different instruments and platforms. The aim is to assess the quality of these data sets and to identify the main sources of uncertainty. The results are presented in a series of tables and figures. The main findings are that the quality of the data is generally good, but that there are significant differences between the different instruments and platforms. The main sources of uncertainty are identified and discussed. The results are used to develop a set of quality assurance metrics and to identify the main areas for improvement.

GAIA-CLIM Report / Deliverable D3.2

Gap Analysis for Integrated Atmospheric ECV Climate Monitoring:

Generic metrology aspects of an atmospheric composition measurement and of data comparisons

Abstract. This report presents the results of a gap analysis for the integrated atmospheric ECV climate monitoring. The main findings are that the current state of the art is not sufficient to meet the requirements of the GAIA-CLIM mission. The main areas for improvement are identified and discussed. The results are used to develop a set of quality assurance metrics and to identify the main areas for improvement.

QA4ECV Report / Deliverable D2.5

QA4ECV

Quality Assurance for Essential Climate Variables

Prototyping QA/Validation Service for Atmospheric ECV Precursors

Detailed Processing Model Version 2

June 2016

Lead by: BIRA-IASB (#2)

Report

PU

Abstract. Many applications and climate data sets require the use of quality assurance metrics and validation procedures. The QA4ECV project is a multi-partner effort to develop a set of quality assurance metrics and validation procedures for atmospheric ECV precursors. The main findings are that the current state of the art is not sufficient to meet the requirements of the GAIA-CLIM mission. The main areas for improvement are identified and discussed. The results are used to develop a set of quality assurance metrics and to identify the main areas for improvement.

Cross GEOS/ cross-EO domains Cal/Val harmonization

Prototyping in Multi-TASTE and ESA CCI_Ozone

Community feedback & endorsement

Implementation and continuous development in FP7 QA4ECV, H2020 GAIA-CLIM, Envisat QWGs, ISSI Cross-EO Val., CCI+/C3S ozone, Sentinel-5p MPC

Lambert et al., JAS 1999, ISSI 2012
Keppens et al., AMT 2015, 2018
Langerock et al., GMD 2015
Verhoelst et al., AMT 2015, EC TN 2016
Hubert et al., AMT 2016
Compernelle et al., EC TN 2017



S5P TROPOMI validation and FRM programme contribute further progress in:

- **Harmonisation of validation practices across networks**
- **Harmonisation of validation reporting across species**
- **Harmonisation of unified error/uncertainty reporting**
- **Validation of ex-ante satellite uncertainties**
- **Criteria of compliance with user/mission requirements**



Atmospheric Chemistry and Physics
An interactive open-access journal of the European Geosciences Union

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Special issue | TROPOMI on Sentinel-5 Precursor: first year in operation (AMT/ACP inter-journal SI)

Editor(s): J. Joiner, B. Veihelmann, D. Loyola, H. Worden, J. Kim, H. Boesch, P. Levelt, I. Aden, and T. Röckmann
Special issue jointly organized between Atmospheric Measurement Techniques and Atmospheric Chemistry and Physics

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Special issues
Special issue | Towards Unified Error Reporting (TUNER)

Editor(s): E. van Damme, D. Ogerstein, N. Livesey, and H. Worden

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Special issues
Special issue | Twenty-five years of operations of the Network for the Detection of Atmospheric Composition Change (NDACC) (AMT/ACP/ESD inter-journal SI) (AMT/ACP/ESD inter-journal SI)

Editor(s): V.H. Freeth, G. Brasseur, C. Zahner, H. Maring, and G. Sillor
Special issue jointly organized between Atmospheric Measurement Techniques, Atmospheric Chemistry and Physics, and Earth System Science Data

SPARC | **GLOBAL STRATOSPHERE WATCH** | **International Ozone Commission**

SPARC/IO3C/GAW Report on Long-term Ozone Trends and Uncertainties in the Stratosphere

I. Petropavichik, S. Godek Benckman, D. Habert, R. Damadeo, B. Hader, K. Sofonea

LOTUS

WCRP



Lambert *et al.*, JAS 1999, ISSI 2012
Keppens *et al.*, AMT 2015, 2018, **2019**
Langerock *et al.*, GMD 2015
Verhoelst *et al.*, AMT 2015, EC TN 2016, **AMT 2020**
Hubert *et al.*, AMT 2016, **LOTUS 2019, AMT 2020**
Compennolle *et al.*, EC TN 2017, **ACP 2019, AMT 2020**
Vigouroux *et al.*, **AMT 2020**



Satellite data uncertainties and QA/QC:

- State-of-the-art ex-ante uncertainties required for a successful validation
- Efficient Quality Control of Level-1b and Level-2 data production necessary before validation can start

FRMs (and other validation data):

- FRM data: fitness-for-purpose (representativeness, influence quantities...), reliable error bars
- FRM data streams: timeliness, sustainability, QA/QC of FRM streams (e.g., issue of ozonesonde network drop since 2016)
- Cooperation with ground-based networks fruitful
- Satellite-to-satellite to capture features and patterns like striping, sea/ice and cloud related outliers...
- Ancillary data: for changes in coordinates, end-to-end validation of retrieval... ⇒ campaigns, supersites
- Data governance (and acknowledgment, licence, redistribution etc.) is a key issue !
- Satellite perspective on FRM data developments: e.g., (why) is the lack of FRM sites in Africa a problem?
- Agreements necessary for guarantying access to national in situ/RS data

Validation methods and tools:

- Harmonized, state-of-the-art, fit-for-purpose validation methods still in development
- Challenges of high resolution validation (e.g. Sentinel-5p at 3.5 x 5.5 km²)
- Propagation of satellite and FRM uncertainties along data harmonization and validation chains
- Closure of comparison error budget, including co-location mismatch errors
- Verification of compliance with mission/user requirements not straightforward
- Full traceability (documentation) of validation data and of validation process

Additional challenges for GEO missions:

- Change in paradigm w.r.t. LEO: diurnal cycle, VZA, SZA, BRDF ("directional accuracy")...
- LEO-AQ satellites as "travelling standards" for GEO-AQ validation ⇒ implementation TBD

Recommendations

- Consistently perform intensive campaigns dedicated to the validation of the capability of the Geo-AQ missions to observe the diurnal cycle of the target species. Such campaigns are conducted at several supersites within each Geo-AQ mission domain where a comprehensive suite of correlative reference measurements is made and a comprehensive set of auxiliary data from a variety of sources is exploited.
- Conduct joint validation campaigns with exchange of reference airborne and ground-based instruments.
- Further develop and eventually apply approaches to the radiometric inter-calibration of the Geo-AQ missions, based on comparisons of Earth radiance data acquired over known targets, SI-traceable test sites where available, precise and approximate ray matching between GEO and LEO pairs of missions, and by taking the LEO missions as a travelling standard. These activities should be pursued within the frame of the WMO GSICS initiative.
- Further develop and eventually apply approaches to the inter-calibration of the Level-2 products of the Geo-AQ missions. These approaches include the comparison of products with inter-calibrated ground-based network data, cross-validation of Level-2 algorithms by exchanging Level-1b data, comparing zonal mean values of the stratospheric sub-column in the Level-2 ozone products, and taking validated LEO missions as a travelling standard.
- Systematically process the Level-2 Constellation Products of the Geo-AQ missions, using one selected common algorithm per Constellation Product.
- Further pursue the harmonization of the reference data used for validation and inter-mission consistency verification of Level-2 products, aiming at common measurement protocols, common QA protocols, common data formats, harmonized data policy and open access.
- Implement a data centre for storage and exchange of all validation data collected for the Geo-AQ missions. Make these data accessible to the entire community involved in the validation of the Geo-AQ mission products and their inter-mission consistency, very soon after acquisition.
- Implement a coordinating unit for ensuring the consistency of the approach and the metrics used for validating the Geo-AQ mission products and their inter-mission consistency.

in-depth validation campaigns essential

exhaustive pre-launch calibration essential

FRM-based satellite-to-satellite alternative retrievals

internal coherence of product families

round-robin to agree on constellation algorithm

sustained FRM programme

EVDC successful harmonisation of validation to be continued

