





Sentinel-5p Operational Validation

Status, lessons and perspectives for GEO-AQ and Sentinel-5

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Sentinel-5p Operational Validation: The people

Product Validation Coordinators: 8

• Core team: 24

Regular contributors: 45

Citation	Quarterly Validation Report of the Copernicus Sentinel-5 Precursor Operational Data Products – #03: July 2018 – May 2019. Lambert, JC., A. Keppens, D. Hubert, B. Langerock, KU. Eichmann, Q. Kleipool, M. Sneep, T. Verhoelst, T. Wagner, M. Weber, C. Ahn, A. Argyrouli, D. Balis, K.L. Chan, S. Compernolle, I. De Smedt, H. Eskes, A.M. Fjæraa, K. Garane, J.F. Gleason, F. Goutail, J. Granville, P. Hedelt, KP. Heue, G. Jaross, ML. Koukouli, J. Landgraf, R. Lutz, S. Niemeier, A. Pazmiño, G. Pinardi, JP. Pommereau, A. Richter, N. Rozemeijer, M.K. Sha, D. Stein Zweers, N. Theys, G. Tilstra, O. Torres, P. Valks, C. Vigouroux, and P. Wang. S5P MPC Routine Operations Consolidated Validation Report series, Issue #03, Version 03.0.1, 126 pp., June 2019.		
Approval Record			
Checked by:	JC. Lambert (BIRA-IASB) Q. L. Kleipool (KNMI) D. Loyola (DLR) J. P. Veefkind (KNMI) A. Dehn (ESA)	MPC ESL-VAL Lead MPC ESL-L1 Lead MPC ESL-L2 Lead MPC Technical Manager MPC Project Officer	
Approved by:	A. Dehn (ESA)	ESA Data Quality Manager	

opernicus Cal/Val Organisation for the Sentinels Cesa

ESA Validation



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 Mission Performance Center

The Mission Performance Center is in charge of the operational and overall validation providing the synthesis of the results.

MPC S1, MPC S2, MPC S3, MPC S5P have been set up.

Quality Working Group QWG

ESA Data Quality Manager

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.

Data Centre

The validation team complete the MPC activities by providing independent validation measurements or independent analysis.

The Sentinel Validation Teams (SVT):

S2VT, S3VT, S5PVT have been set up.

Fiducial Reference Measurements providers

Specific activities need to be put in place for providing mandatory FRMs (e.g. for atmospheric FRMs:

PANDONIA/PGN, FRM4DOAS, FRM4GHG)

User Community and international forum:

The validation program benefits from the feedback from:

- Workshops/conferences (ESA or international)
- Bilateral relation (NASA, NOAA, CNES, DLR, UKSA, JRC, EUMETSAT etc.)
- Coordination within **CEOS WGCV** and **CEOS VCs**

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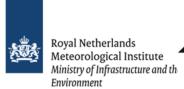




opernicus S5P Mission Performance Centre (MPC)



Funding: EC/ESA + national NL/NSO, D/DLR, BE/BELSPO

















Objectives + Responsibilities

Routine Quality Control

Level 1 and Level 2

Long-Term Monitoring

TROPOMI instrument sensor and ageing

In-flight calibration

TROPOMI instrument on-board S5P – meet product quality requirements

Geophysical Validation of Products

Using external and independent data sets on a routine basis

Maintenance and evolution

Manage the updates of:

- Calibration algorithms and tools
- L1 and L2 Processor algorithms
- Quality control tools
- Validation algorithms

Communication S5P/TROPOMI status and products

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Sentinel-5p Routine Operations Validation Service

S5P Mission Performance Centre (MPC) to provide service-based solution for Routine Operations validation:

- Automated, routine comparison of S5P data vs. FRMs
- S5P validation database for in-depth MPC studies
- Automated generation of quick-look comparison reports

- Monitoring of S5P products health
- Public and MPC quality information on S5P products
- Support to L1/L2 algorithm evolution
- Synthesis with S5PVT results, ECMWF/CAMS, literature...



















Validation Data Streams into VDAF

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, MAX-DOAS, Pandonia		
L2_O3_P	R O ₃ profile (incl. troposphere)	ozonesonde, stratospheric DIAL, tropospheric DIAL		
L2_O3_T0	CL O ₃ tropospheric column	ozonesonde		
	NO ₂ stratospheric column	ZSL-DOAS		
L2_NO2	NO ₂ tropospheric column	MAX-DOAS		
	NO ₂ total column	<u>Pandonia</u>		
L2_SO2	SO ₂ total column	MAX-DOAS, Pandonia		
L2_HCH	HCHO total column	MAX-DOAS, Pandonia		
L2_CO	CO total column	TCCON FTIR (NIR), NDACC FTIR (MIR)		
L2_CH4	CH ₄ total column	TCCON FTIR (NIR), NDACC FTIR (MIR)		
	Cloud Fraction	not available		
L2_CLOU	Cloud Height (pressure)	Cloudnet lidar/radar		
	Cloud Optical Thickness	not available		
12 450	UV Aerosol Absorbing Index	not available		
L2_AER	Aerosol Layer Height	EARLINET aerosol lidar, EUMETNET/ALC ceilometer		











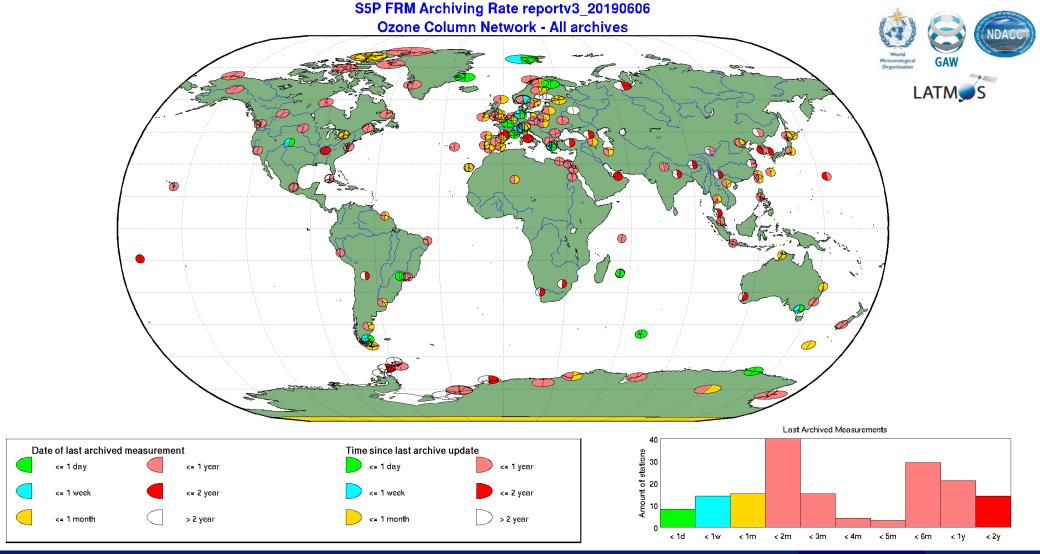






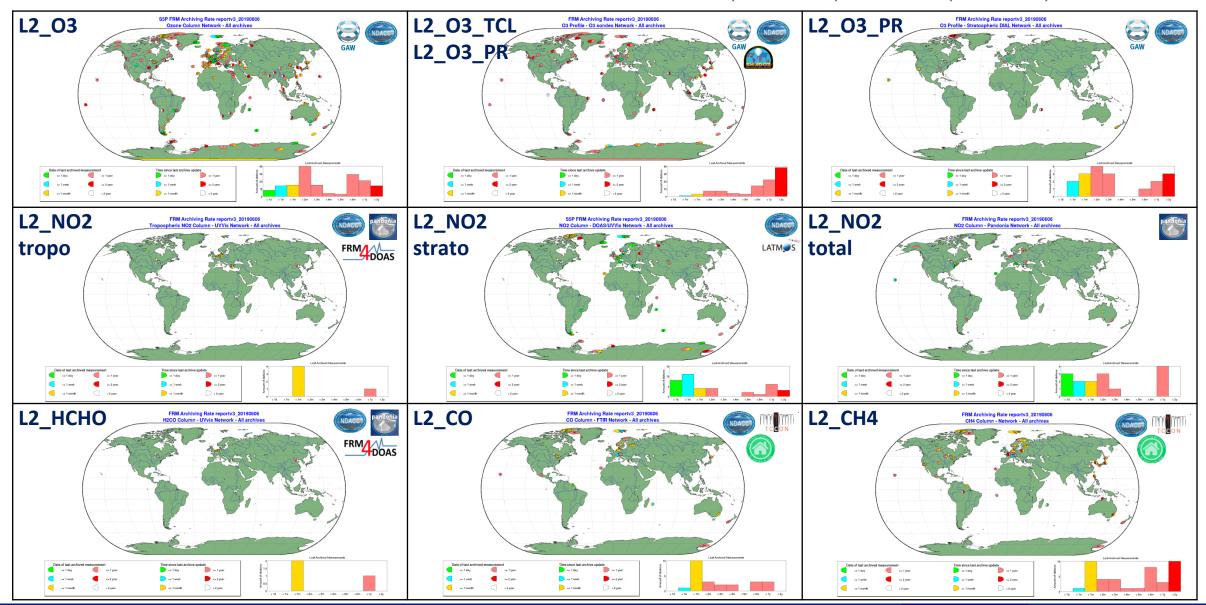
Status of FRM / Validation Data Streams

O3 column data from LATMOS_RT (ZSL-DOAS/SAOZ), NDACC DHF (ZSL-DOAS) and WMO/GAW WOUDC (Brewer, Dobson, ZSL-DOAS) collected via CORR-2/Multi-TASTE (BIRA-IASB) and EVDC (NILU)



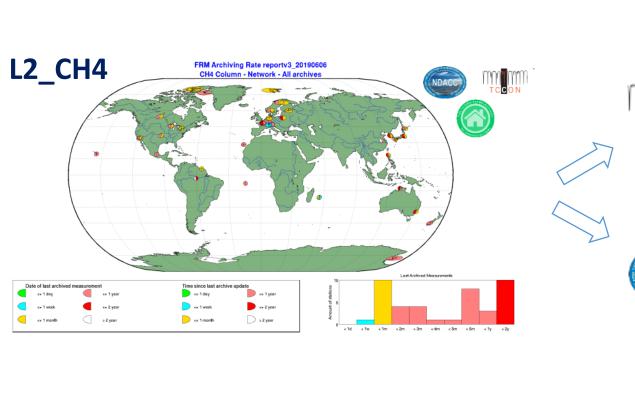
Status of FRM and other Validation Data Streams

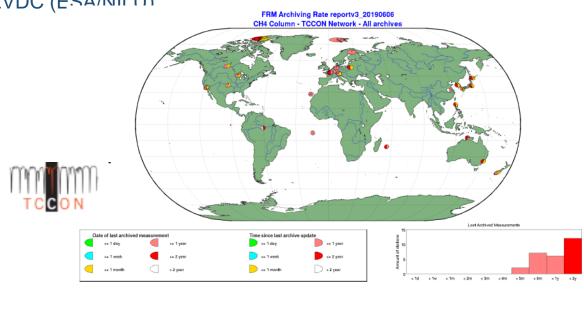
from NDACC, PGN, SHADOZ, TCCON and WOUDC collected via CORR-2 (BIRA-IASB) and EVDC (ESA/NILU)

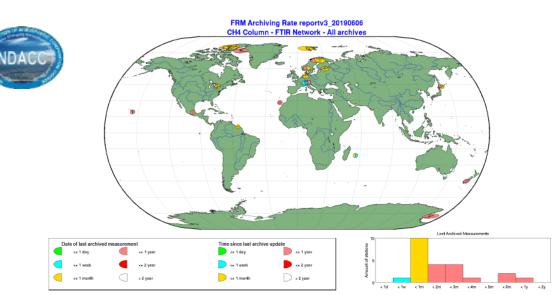


Details of CH4 Validation Data Streams

from NDACC DHF and TCCON via CORR-2 (BIRA-IASB) and EVDC (ESA/NII II)







Generic validation chain, state-of-the-art co-locators, harmonized terminology, agreed metrics...

Atmos. Meas. Tech., 8, 2093-2120, 2015 www.atmos-meas-tech.net/8/2093/2015 doi:10.5194/amt-8-2093-2015 @ Author(s) 2015. CC Attribution 3.0 License. Atmospheric -

Geosci. Model Dev., 8, 911-921, 2015 www.geosci-model-dev.net/8/911/2019 doi:10.5194/gmd-8-911-2015 @ Author(s) 2015. CC Attribution 3.0 License

Model Dev

Round-robin methodology

A. Keppens1, J.-C. Lar T. Verhoelst1, A. Delclo ¹Belgian Institute for Sp ²Rutherford Appleton L 3Royal Netherlands Met 4Royal Meteorological I ⁵Laboratoire Atmosphère Versailles St-Ouentin-er ⁶Finnish Meteorological ⁷Federal Office of Meteo

⁸European Space Agenc Correspondence to: A.

Received: 16 September Revised: 17 April 2015

Abstract, A methodolo the geophysical validati from nadir UV backsca

Description

model data B. Langerock¹, M.

Belgian institute ²S&T. Olof Palm Correspondence t

Received: 29 Septen Revised: 6 March 20

Abstract, MACC-I

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MACC-II,III/CAMS

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Karl W. Hoppel⁸, Bry C. Thomas McElroy 13 James M. Russell III1 Kevin B. Strawbridge Anne M. Thompson² Peter von der Gathen ¹Royal Belgian Institute Laboratoire de l'Atmo (Université de La Réuni ³Laboratoire de Météoro

(Université Blaise Pasca Institute of Space and A SIstituto di Fisica Applic Jet Propulsion Laborato ⁷Laboratoire Atmosphèr Centre National de la Rea Naval Research Lab. W 9NOAA Earth System Re 10Finnish Meteorological 11 Jet Propulsion Laborat German Aerospace Cen ¹³York University, Toron Department of Earth a 15 Kochi University of Te ¹⁶National Institute for I ¹⁷ National Institute of W ¹⁸Department of Atmost 19CEILAP-UNIDEF (MI

²⁰Research Centre Jülich

Atmos. Meas. Tech., 9, 2497-2534, 2016 www.atmos-meas-tech.net/9/2497/2016/ doi:10.5194/amt-9-2497-2016 @ Author(s) 2016. CC Attribution 3.0 License

Atmos. Meas. Tech., 8, 5039-5062, 2015 www.atmos-meas-tech.net/8/5039/2015/ doi:10.5194/amt-8-5039-2015

Ground-based 14 limb and o

Daan Hubert1, Jean-Ch Adam E. Bourassa⁴, Ug mismatch and smoothing

> ¹Belgian Institute for Space Aeronomy (BIR ²Meteorological Observatory at Hohenpeiße 3Laboratoire Atmosphères, Milieux, Obser ⁴Izaña Atmospheric Research Center, AEM

Received: 23 May 2015 - Published in Atm Revised: 6 November 2015 - Accepted: 11

Abstract. Comparisons with ground-based surements constitute a key component in satellite data on atmospheric composition get of these comparisons contains not only errors but also several terms related to diff pling and smoothing of the inhomogeneou mospheric field. A versatile system for O Simulation Experiments (OSSEs), named used here to quantify these terms. Based o of pragmatic observation operators onto h

mospheric fields, it allows a simulation of measurement, and consequently, also of the differences to be expected from spatial and temporal field variations between both measurements making up a comparison pair. As a topical case study, the system is used to evaluate the error budget of total ozone column (TOC) comparisons between

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Metrology of ground-bas

T. Verhoelst¹, J. Granville¹, F. Hendrick M. Van Roozendael¹, and J.-C. Lamber

Correspondence to: T. Verhoelst (tijl.verh

cantly to the comparison error budget. The detailed analysis of the comparison results, including the metrological errors suggests that the published random measurement uncertainties for GODFITy3 reprocessed satellite data are potentially overestimated, and adjustments are proposed here. This successful application of the OSSSMOSE system to close for the

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



A Horizon 2020 project; Grant

Date: 27 January

Lead Beneficiary

Dissemination lev









QA4ECV Report / Deliverable D2.5

QA4ECV

Quality Assurance for Essential Climate Variables

Prototype QA/Validation Service

for Atmospheric ECV Precursors

Detailed Processing Model



Version 2







Cross GEOSS EO Cal/Val Harmonization



Prototyping in ESA Multi-TASTE and **CCI** Ozone



Community feedback / endorsement







Implemention in FP7 QA4ECV-AVS, H2020 GAIA-CLIM, C3S 312#ozone, S5P MPC VDAF, CAMS-NDACC. CCI+

SSP MPC Operational Validation

Data Handling, Co-location and Comparison Toolset

HARP



harp documentation

HARP Installation Data formats Algorithms Operations Ingestion definitions C library IDL interface Python interface Command line tools

https://cdn.rawgit.com/stcorp/harp/master/doc/html/index.html

Docs » Command line tools

Command line tools

The section describes the command line tools provided by the HARP toolkit.

- harpcheck
- harpcollocate
 - Collocation
 - Obtaining collocation result file
 - Resampling collocation result file
 - Updating collocation result file
- harpconvert
- harpdump
- harpmerge



S5P Data Streams into MPC VDAF

- Overpass data extractor in S5P PDGS
- Based on 3D Observation Operators
- Correction for NO₂ diurnal cycle
- Optimization of data volumes

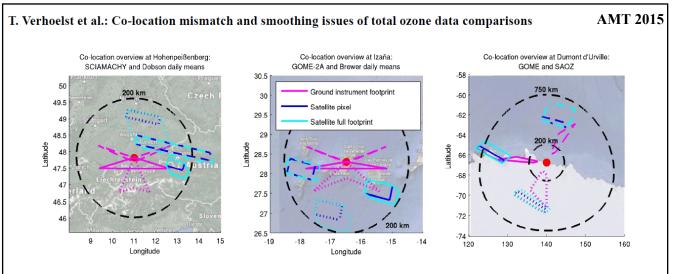
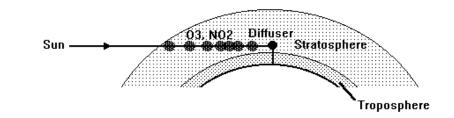
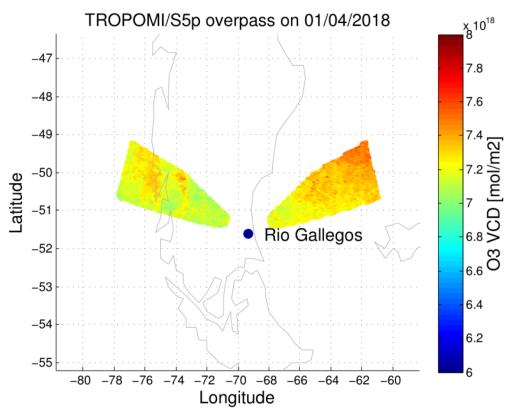
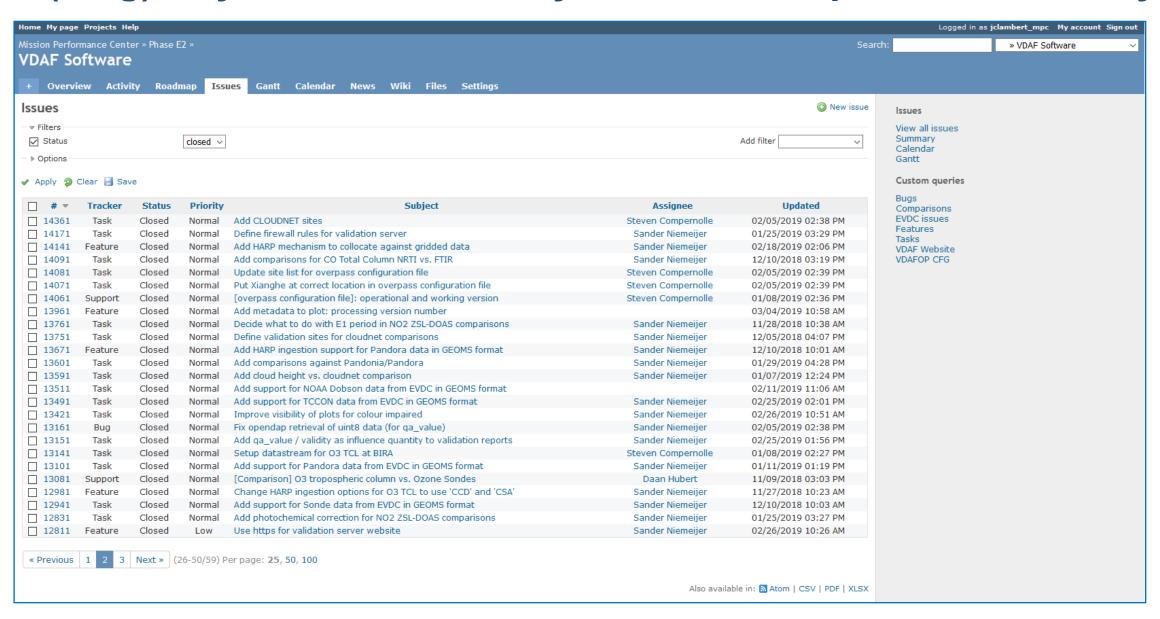


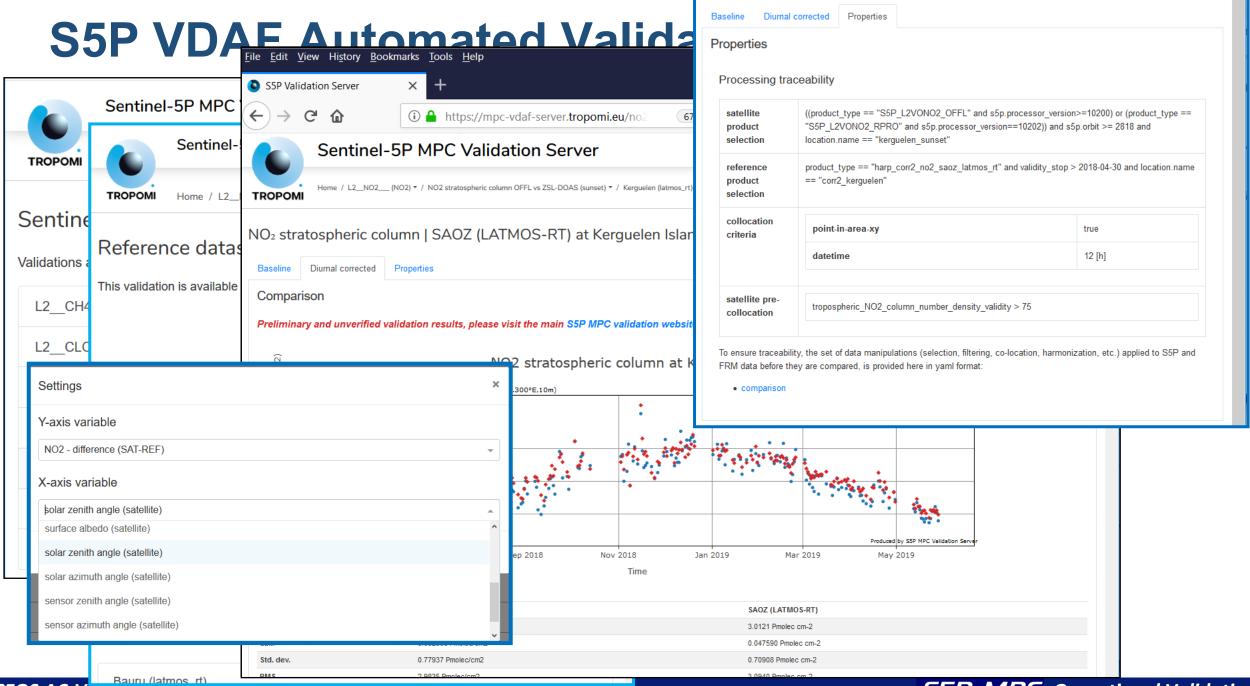
Figure 4. Co-located ground-satellite measurement pairs near summer and winter solstice (dashed and dotted lines, respectively) and near the autumn and spring equinox (solid line). The station is indicated by a red dot, the ground observation operators in magenta, the satellite pixel in dark blue and the full satellite observation operator in cyan.



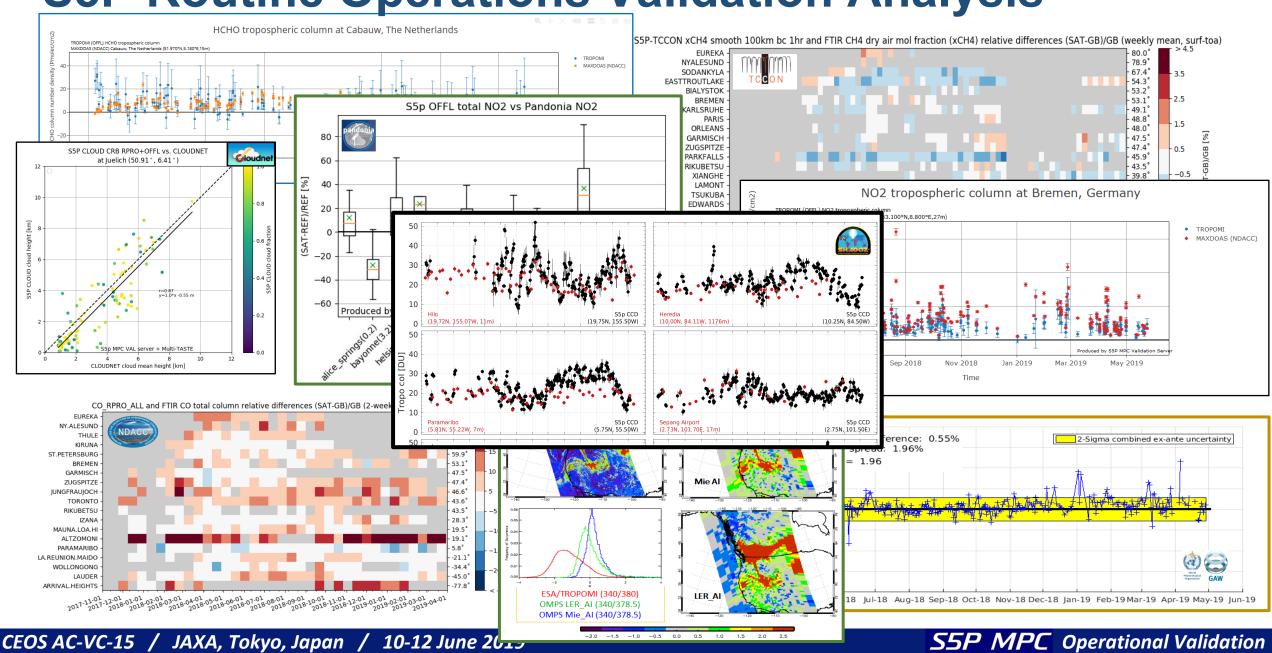


The (long) way from Scientific Systems to an Operational Facility...





S5P Routine Operations Validation Analysis



Public and Internal Outputs



CEOS AC-VC-15

 S5P Routine Operations Consolidated Validation Report
 May 2019
 S5P-MPC-IASB-ROCVR-03.0.1-20190615

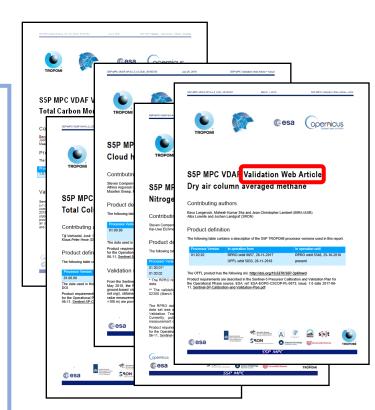
 ROCVR update #03, issue 03.0.1, 2019-06-15
 Page 10 of 126

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:

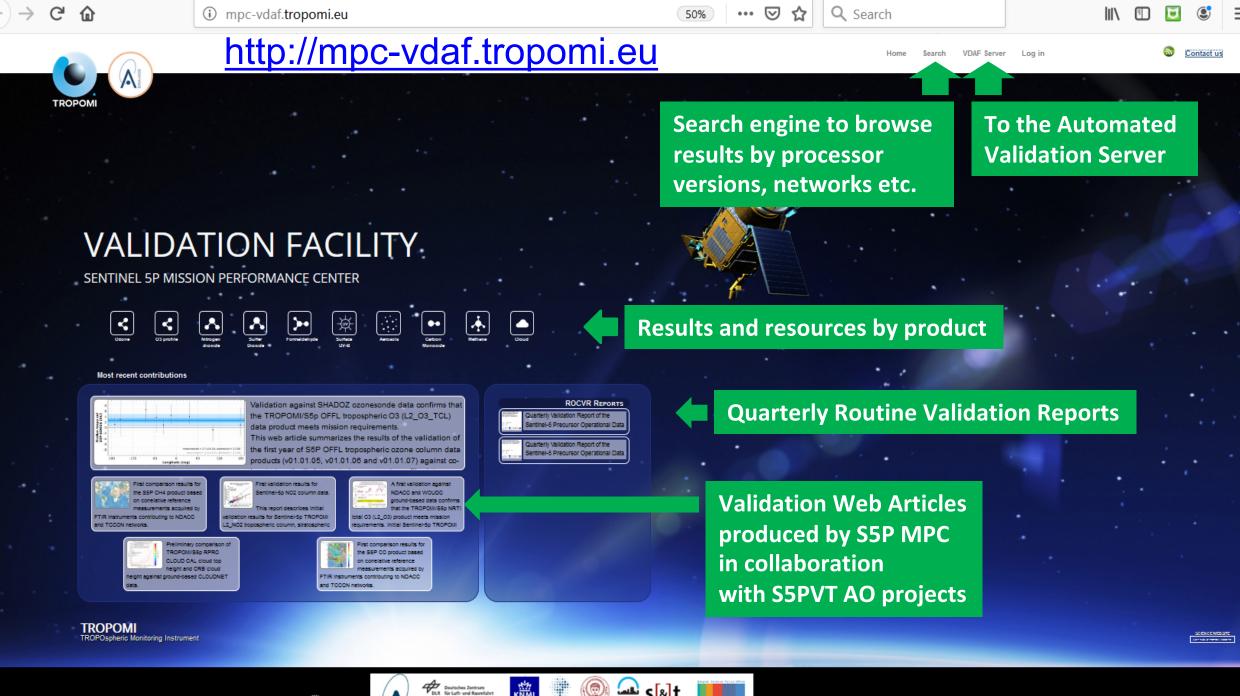
Product ID	Stream	Product	Bias	Dispersion	Special features
L2_O3	NRTI	O ₃ column	1%	2.5%	
	OFFL	O ₃ column	0.4%	2%	
L2_03_TCL	OFFL (CCD)	O ₃ tropospheric column	+14%	23%	Signs of large positive bias during biomass burning conditions. Imprints of sampling-related biases.
L2_NO2	NRTI	NO ₂ troposphere NO ₂ stratosphere	-30% -7%	4 Pmol/cm ² 0.5 Pmol/cm ²	
	OFFL RPRO	NO ₂ troposphere NO ₂ stratosphere	-30% -7%	4 Pmol/cm ² 0.5 Pmol/cm ²	
L2_HCHO	NRTI	HCHO column	-33%	9 Pmol/cm ²	
	OFFL RPRO	HCHO column	-33%	9 Pmol/cm²	
L2 SO2	NRTI	SO ₂ column	0.2 DU	0.2 DU	
L2_302	OFFL	SO ₂ column	0.2 DU	0.2 DU	
[_2_CO	NRTI	CO column	10%	5%	Along track stripes
L2_00	OFFL	CO column	6%	5%	Along track stripes
L2_CH4	OFFL	CH4 column	-0.3	1%	Pixels above inland water are not filtered in qa_value. Remaining outliers with qa_value>0.5
L2_CLOUD	NRTI	CAL CTH CRB CH CAL COT	-15% -20% +7.9 [-]	2 km 1 km	Bias towards the a priori cloud height up to and including 01.01.05. COT bias vs VIIRS.
	OFFL	CAL CTH CRB CH CAL COT	-15% -20% +7.9 [-]	2 km 1 km	Bias towards the a priori cloud height up to and including 01.01.05. COT bias vs VIIRS.
L2_AER_AI	NRTI	aerosol index	-1 Al unit	0.1 Al unit	
	OFFL	aerosol index	-1 Al unit	0.1 Al unit	

Table 2 – Representative quality indicators (bias and dispersion) as estimated from the validation studies of the





S5P MPC Operational Validation



















Status and Lessons Learnt



- S5P MPC Routine Operations validation facility VDAF in service
- In operation: Automated Validation Server, validation analysis consortium, portfolio of outputs, internal and public web-based facilities
- Approach of complementing MPC VDAF/VAL with S5PVT AO activities successful
- Valuable synergies/convergence between Copernicus space (MPC),
 FRM procurement and (CAMS/C3S) service components
- Enhanced coordination desired for approach to/funding for FRM gap analysis, deployment, data generation and delivery





TROPOM

Perspectives for S-5 and GEO-AQ



Critical elements (for single missions):

- FRM data streams: availability, relevance, timeliness, sustainability
- Harmonized, state-of-the-art, fit-for-purpose validation methods
- Propagation of uncertainties, closure of comparison error budget
- Definition and implementation of quality compliance criteria...
- Operationalization and service set-up

Additional challenges for GEO-AQ:

Change in paradigm wrt LEO: diurnal cycle, VZA/SZA, BRDF...

Additional challenges for any constellation:

Inter-mission consistency of validation: methods, metrics, FRMs, AKs...







Perspectives for GEO-AQ

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, 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.
- 4. 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 consistent validation approach and metrics for the Geo-AQ mission products and their inter-mission consistency.

Geostationary Satellite Constellation for Observing Global Air Quality: Geophysical Validation Needs

> Prepared by the CEOS Atmospheric Composition Virtual Constellation and the CEOS Working Group on Calibration and Validation Version 1.0, 24 April 2019

