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Copernicus Sentinel-5 Precursor Routine Validation using Fiducial Reference Measurement data sets

Angelika Dehn (ESA/ESRIN)



- S5P Level 2 Product Requirements
- S5P Cal/Val organization
- Fiducial Reference Measurements (FRM)
 - Definition
 - ESA FRM activities
- S5P routine validation
 - Examples S5P validation based on FRMs

Sentinel-5P Level 2 Product Requirements











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Parameter	Data Product	Vertical Resolution	Bias	Random
Ozone 	Ozone Profile	6 km	30%	10%
	Total Ozone	total column	5%	1.6-2.5%
	Tropospheric Ozone	trop column	25%	10%
NO ₂ 	Stratospheric NO ₂	strat column	<10%	0.5e15
	Tropospheric NO ₂	trop column	50%	0.7e15
SO ₂ 	SO ₂ enhanced	total column	30%	0.15-0.3 (0.06-0.12) DU
	Total SO ₂	total column	50%	1-3 (0.4-1.2) DU
Formaldehyde 	Total HCHO	total column	80%	1.2e16 (4e15)
CO 	Total CO	total column	15%	<10%
Methane 	Total CH ₄	total column	1.5%	1%
Cloud 	Cloud Fraction	total column	<20%	0.05
	Albedo (Optical Thickness)	total column	<20%	0.05 (10)
	Cloud Height (Pressure)	total column	<20%	<0.5 km (<30hPa)
Aerosol 	Aerosol Layer Height	total column	<100hPa	<50hPa
	Aerosol Type	total column	~1 AAI	<0.1 AAI
Surface UV	Provided by FMI in frame of the Finnish Sentinel Collaborative Ground Segment			

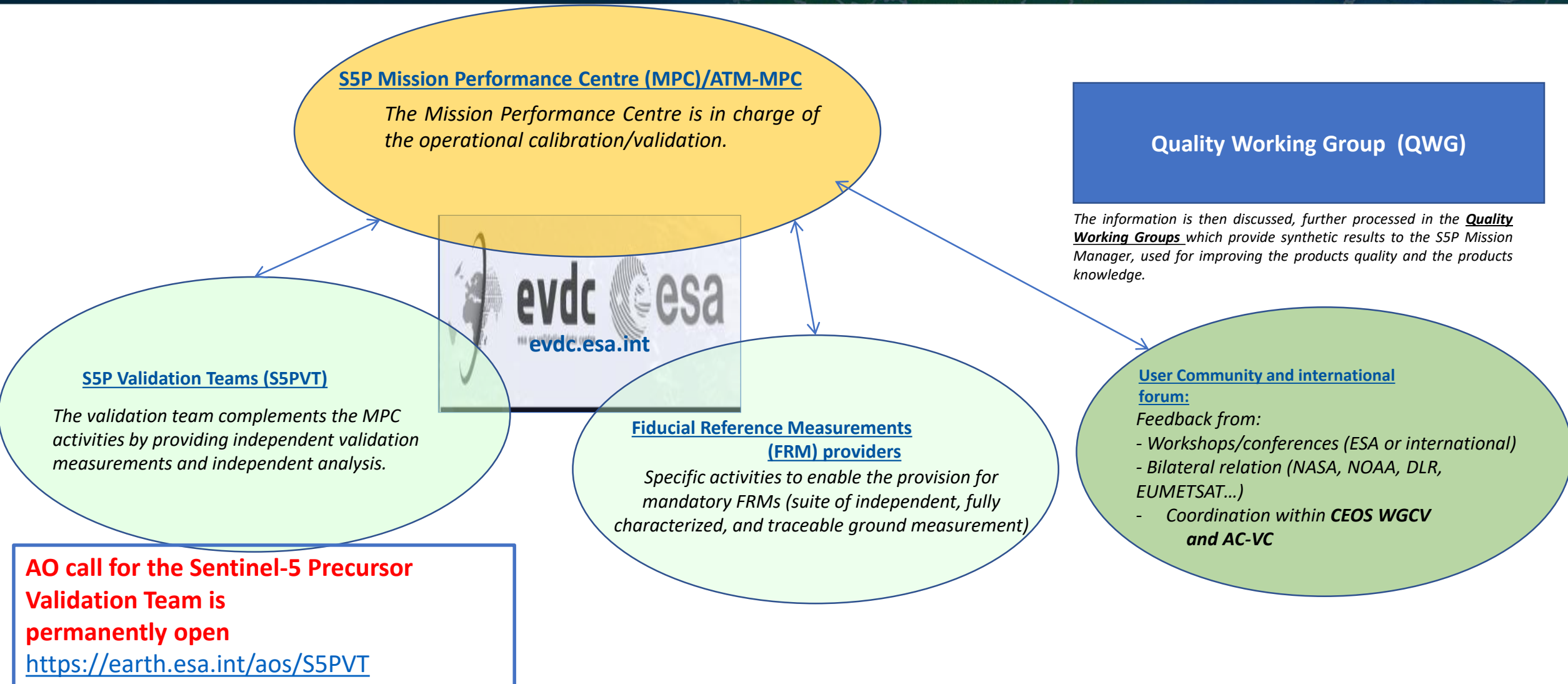
Sentinel-5P Cal/Val Organization



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Fiducial Reference Measurements



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Fiducial Reference Measurements (FRM) definition:

• *“The suite of independent **tailored and fully characterised** measurements that provide the maximum Return On Investment (ROI) for a satellite mission by delivering, to users, the required confidence in data products, in the form of independent validation results and satellite measurement uncertainty estimation, over the entire end-to-end duration of a satellite mission.”*

FRM characteristics

- FRM measurements - ideally have **documented SI traceability** (e.g. via round-robin characterisation and regular pre-and post deployment calibration of instruments) using metrology standards and/or community recognised best practices;
- FRM measurements are **independent** from the satellite geophysical retrieval process;
- An **uncertainty budget** for all FRM instruments, and derived measurements, is available and maintained;
- FRM measurement **protocols, procedures** and community-wide management practices (measurement, processing, archive, documents, etc.) are defined, published and adhered to by FRM instrument deployments;
- FRM are **accessible** to other researchers allowing independent verification of processing systems;
- FRM are **required** to determine the on-orbit uncertainty characteristics of satellite geophysical measurements via independent validation activities.

Pandonia-Global-Network



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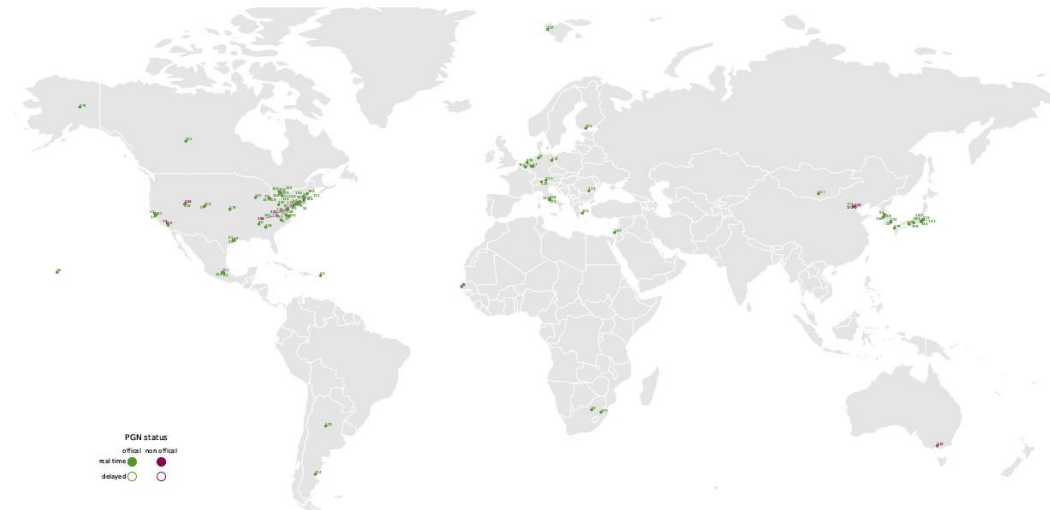


<https://www.pandonia-global-network.org/>

- Ground-based remote sensing network using Pandora-2S and Pandora spectrometers
- Purpose: achieve long, uninterrupted, well-maintained, homogeneously calibrated Time-series of ground-based remote sensing atmospheric measurements:
Target products:
 - total & tropospheric column: O₃, NO₂
 - additional products: SO₂, HCHO, aerosol
- PGN ESA/NASA collaboration
Established in 2018



PGN stations distribution by 30th May 2022.



PGN status
official non-official
mal time delayed

127 official instruments

01 AigueTX	65 Alzomora*	189 Anmyeon	119 Athens-NOA	158 AtlantaGA*	213 Bangkok*	38 BayonneNJ	172 Beijing*	171 Beijing-RAD	112 Berlin
188 Braunschweig*	155 BoulderMA	07 BoulderCO	204 BoulderCO-NCAR	21 Bremen	128 BristolPA	112 Braunschweig	180 Brooklyn	160 Brasov-Sicce	111 Bucharest
204 BuffaloNY	30 Busan	118 Cabauw	26 CambridgeMA*	184 CapeElizabethME	70 ChapelHillNC	31 CharlesCityVA	223 ColumbiaMD*	134 Comandreshivadavia	148 Curitiba-PELAB
123 Corrida	88 Dakar	217 DanaoIsland	150 Davis	38 Daquanzhou	106 Downsview*	185 EastProvidenceRI	109 Eggen	146 Eureka-PELAB	141 HamptonVA-HU
174 FairbanksAK	50 Fajardo*	107 Fang	35 ForestParkMO	127 FortMeKay	23 FourCornersNM	118 Fukuroka	59 GreenvilleMD*	27 HamptonVA	61 LaPorteTX*
101 Helsinki	25 HoustonTX	64 HuntsvilleAL	201 Incheon-ES	110 Innsbruck	121 Innsbruck-FCS*	30 Juellch	167 KnoxvilleTN	198 Kobe	157 Nagoya
181 LondonderryNH	181 LynnMA	188 MadisonCT	178 MauiHawaii	135 ManhattanNY-CCNY	96 MauiKauaiHI	140 MexicoCity-UNAM	157 MexicoCity-Valde	14 MountainViewCA	55 QueensNY
69 NewBrunswickNJ	64 NewHavenCT	235 NewLondonCT	152 NyAlesund	51 OldFarmsNY	166 PhiladelphiaPA	187 PittsburghPA	53 Potchefstroom*	51 RichmondCA	51 RichmondCA
118 RomeCA	112 Rome-GAP	117 Rome-GAP	147 SWDrosolMI	164 SaultSteMarieUT	101 SarajevoCA	50 Saitama*	150 Sapporo*	164 Seosan	54 Seoul
148 Seoul-SNU	126 Shijiazhuang	139 SouthJordanUT	109 StGeorge	103 StonyPlain	182 Tai-Aviv	194 Tokyo-TMU	145 Toronto-Scarborough	108 Toronto-West	193 Tsukuba
175 Tsukuba-NIES	110 Tsukuba-NIES-West	236 Ulaanbaatar	216 Ulaanbaatar	150 Ulsan	159 Wakenroom	140 WashingtonDC	177 WestportCT	208 Windsor-West	68 WinghamWoodCA
161 Xianghe	146 Yokosuka	191 Yongin							

*more than one instrument

20220530



PGN station distribution May 2022

<http://frm4doas.aeronomie.be>

FRM4DOAS 1 during 2016-2020

- Harmonization of retrievals from UV-Vis ground based spectrometers (e.g. MAXDOAS):
 - Specification of best practices for instrument operation
 - Support to preparation of the CINDI-2 campaign
 - Round Robin comparison of algorithms
 - Development of centralised processing system
- Target products:
troposph. & stratosph. NO₂ vertical profiles, total O₃ and trop. HCHO profile
- Preparation for operational readiness of FRM4DOAS central processing
 - Establishment of data flow to NDACC and EVDC databases
 - Algorithm optimisation

FRM4DOAS 2 during 2021-2025

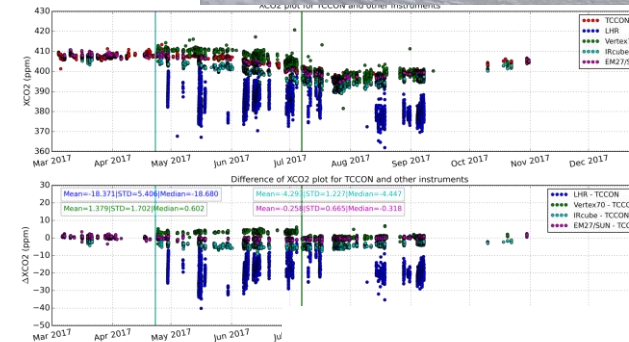
- Consolidation of stratospheric NO₂ product
- Development of a NRT cloud product
- Development of MAX-DOAS aerosol product
- Development of advanced urban tropospheric NO₂ product



<http://frm4ghg.aeronomie.be>

FRM4GHG 1 during 2016-2020

- Inter-comparison of ground based transportable FTIR systems with reference to TCCON as standard system – measurement campaign in Sodankyla/Finland
- provide a guideline for further development of new observation sites to complement the TCCON network
- Target Products: CO, CH₄



FRM4GHG 2 during 2021-2025

- Improve instruments (e.g. solar tracker)
- Evolve algorithms
- Address network harmonization (TCCON and COCCON) (e.g. travel standard)

Intercomparison of low and high resolution infrared spectrometers for ground-based solar remote sensing measurements of total column concentrations of CO₂, CH₄ and CO

Mahesh Kumar Sha¹, Martine De Mazière¹, Justus Notholt², Thomas Blumenstock³, Huilin Chen⁴, Angelika Dehn⁵, David W T Griffith⁶, Frank Hase³, Pauli Heikkinen⁷, Christian Hermans¹, Alex Hoffmann⁸, Marko Huebner⁸, Nicholas Jones⁹, Rigel Kivi⁷, Bavo Langerock¹, Christof Petri², Francis Scolas¹, Qiansi Tu², and Damien Weidmann⁸

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³Karlsruhe Institute of Technology, IMK-ASF, Karlsruhe, Germany
⁴Centre for Isotope Research, University of Groningen, Groningen, The Netherlands
⁵European Space Agency, ESA/ESRIN
⁶University of Wollongong, Wollongong, Australia
⁷Finnish Meteorological Institute, Sodankylä, Finland
⁸Rutherford Appleton Laboratory, United Kingdom

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Paper submission AMT:

FRM development and operation – COCCON



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<https://www.imk-asf.kit.edu/english/COCCON.php>

KIT (Karlsruhe Institute for Technology)

COCCON PROCEEDS: September 2017 – March 2023:

FTIR spectrometer EM27/SUN –

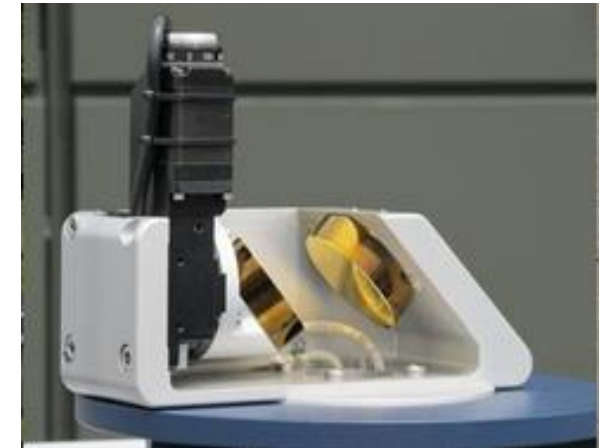
Prototype for centralised data collection and processing facility at KIT (Karlsruhe)

Objectives:

- CO, CO₂, CH₄ Spectra generation from the raw interferograms
- Perform a quality screening for discarding invalid spectra
- Create a web interface and a storage facility
- Demonstration of the validity of the workflow and of the generated spectra by performing a quantitative spectral analysis (retrieval of column-averaged trace gas abundances from a test set of uploaded spectra)

Operational contract **COCCON OPERA** 2023 - 2027

- Network processing Operations and R&D



ESA planned FRM activities (related to S5p)



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ESA open tenders (funded through Copernicus):

2023-2027

FRM support in scope for S5p validation for 4 years duration:

- i) **GHG ground based FTIR/TCCON**
- ii) **FRM4DOAS operational implementation**
(central processing, harmonised data sets)

EVDC - ESA atmospheric Validation Data Centre



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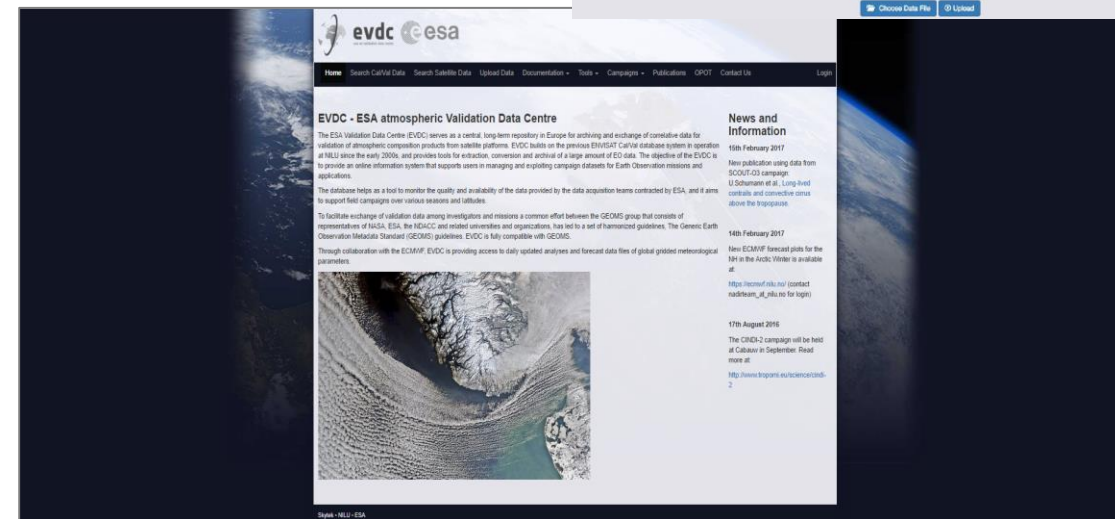
Official ESA repository for validation and campaign datasets, including FRM.

S5P MPC to access FRM and other validation data sets via the EVDC.








S5PVT to upload AO validation data sets to the EVDC.

<https://evdc.esa.int>

- Overpass predictor and Orbit Tool;
- Satellite data sub-setting: S5p, Aeolus, MIPAS
- GEOMS format support tools
- DOI support
- Coordination of GEOMS and DCIO meetings including NDACC, WOUDC
- Evolution for EarthCare functionalities



Fiducial Reference Measurements and other validation data

S5P Data Product	Mission Requirements		Fiducial Reference Measurements and other Validation Data Sources	Satellite Measurements
	Systematic	Random		
 O ₃ total column	5%	2.5%	Brewer, Dobson, ZSL-DOAS, PGN	OMI, GOME-2
 O ₃ vertical profile	30%	10%	ozonesonde, lidar (DIAL), tropo DIAL	OMI, GOME-2
 O ₃ tropospheric column	25%	25%	ozonesonde	OMI, GOME-2
 NO ₂ stratospheric column	10%	0.5 e15	NDACC/ZSL-DOAS	OMI, GOME-2
 NO ₂ tropospheric column	50%	0.7 e15	MAX-DOAS	OMI, GOME-2
 NO ₂ total column	-	-	PGN/Pandonia	OMI, GOME-2
 SO ₂ total column	30%	30%	MAX-DOAS, PGN/Pandonia	OMI, GOME-2, OMPS
HCHO total column	80%	1.2 e16	MAX-DOAS, NDACC FTIR, PGN	OMI, GOME-2
CO total column	15%	10%	NDACC/FTIR, TCCON, COCCON	GOSAT, OCO
CH ₄ total column	1.5%	1%	NDACC/FTIR, TCCON, COCCON	GOSAT, OCO
Cloud Fraction	20%	0.05	FRM not available	VIIRS, OMI, GOME-2
Cloud Height (pressure)	20%	0.5 km	Cloudnet lidar/radar	VIIRS, OMI, GOME-2
Cloud Optical Thickness	20%	0.05	FRM not available	VIIRS, OMI, GOME-2
Aerosol Absorbing Index	1 AAI	0.1 AAI	FRM not available	OMI, OMPS-NP
Aerosol Layer Height	100 hPa	50 hPa	EARLINET lidar, EUMETNET ceilometer	CALIPSO, VIIRS



Status May 2022

Colour code: **automated production** **manual validation, automated production in development**
quality evaluation mainly via diagnostics and satellite data intercomparisons

Courtesy, ATM- MPC
BIRA-IASB

Sentinel-5P Level 2 Product Assessment



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Copernicus Atmospheric Mission Performance Cluster Service

Quarterly Validation Report of the Copernicus Sentinel-5 Precursor Operational Data Products #16: April 2018 – August 2022

Prepared by Copernicus Atmospheric Mission Performance Cluster Service
 Reference SSP-MPC-IASB-ROCVR-16.01.00-20220923
 CI identification DI-MPC-ROCVR / TD-VALREP
 Document update #16
 Issue 16.01.00
 Date of issue 23 September 2022
 Status Final
 Distribution Public



Representative Quality Indicators

Representative values of key quality indicators (bias and dispersion vs. reference measurements, and special features) have been derived for the following S5P operational data products on the basis of the validation results reported in this document:

Product ID	Stream	Product	Bias	Dispersion	Special features
L2_O3	NRTI	O ₃ column	0.8 %	2.5 %	Larger dispersion over snow/ice due to coarse surface albedo climatology (up to but excluding v02.01.xx, which has a dynamic determination of surface albedo). Potentially some increase in overall bias (+0.7%) since v02.02.01 (5 July 2021).
	OFFL	O ₃ column	0.3 %	2 %	Some increase in overall bias (+0.5 to +1.5%) since v02.02.01 (1 July 2021).
L2_O3_TCL	OFFL (CCD)	O ₃ tropospheric column	+17 %	26 %	Geographical imprints of sampling-related biases. Seasonal change of the bias. More elevated positive bias in Atlantic region during biomass burning season.
L2_O3_PR	NRTI	O ₃ profile	10 %	5-20 %	Bias below 10 % in the troposphere up to UTLS, and higher dispersion. Vertically oscillating bias of 5-10 % (positive to negative) in the stratosphere, with a smaller dispersion.
	OFFL	O ₃ profile	10 %	5-20 %	
L2_NO2	NRTI	NO ₂ troposphere NO ₂ stratosphere NO ₂ total	-37% -5% 0±50%	2.6 Pmolec/cm ² 0.3 Pmolec/cm ² -	The bias and dispersion sorted by column amount: Troposphere [<2 Pmolec/cm ²] +18% (0.7 Pmolec/cm ²), [>15 Pmolec/cm ²] -46% (7.3 Pmolec/cm ²). Total [\pm 6 Pmolec/cm ²]: +3% (0.1 Pmolec/cm ²) and -18% (1.9 Pmolec/cm ²). The products improve for later versions, e.g. VDAF-AVS tropospheric bias decreases to -16% for the PAL reprocessed data.
	OFFL RPRO	NO ₂ troposphere NO ₂ stratosphere NO ₂ total	-34% -5% -7%	2.6 Pmolec/cm ² 0.3 Pmolec/cm ² 1.5 Pmolec/cm ²	
L2_HCHO	NRTI	HCHO, low	+28%	9 Pmolec/cm ²	Bias and dispersion depend on column amount: [<2.5 Pmolec/cm ²] positive bias, low dispersion, [>8 Pmolec/cm ²] negative bias, high dispersion.
	OFFL RPRO	HCHO, high	-29%	25 Pmolec/cm ²	
L2_SO2	NRTI	SO ₂ column	0.2 DU	0.2 DU	Lack of validation stations 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. Processor update on July 1, 2021 introduces a de-striped product and a change in spectroscopic parameters. Preliminary results indicate that the bias reduces to 2.9%.
	OFFL	CO column	6.5% before July 2021 2.9% after July 2021	5%	

<http://mpc-vdaf.tropomi.eu/>

- Routine Product Validation by the ATM – Mission Performance Cluster
- Quarterly reports contains summary about Quality indicators

Product ID	Stream	Product	Bias	Dispersion	Special features
L2_CH4	OFFL	CH4 column	-0.03%	0.63%	Along orbit stripes. Underestimation at low albedo. Remaining outliers with qa_value > 0.5. 1-4% seasonal and SZA dependence of bias. Lower amount of pixels with qa_value > 0.5 between March 11 2020 and July 1 2021 due to changed cloud data. Processor update on November 14 2021 produces data over the ocean (sun-glint), updated spectroscopy, a-posteriori bias correction independent of any reference data.
L2_CLOUD	NRTI OFFL	CALv1 CTH (h)	-30%	2 km	Low clouds (l): CLOUDNET CTH < 4km; high clouds (h): CLOUDNET CTH > 4km. Snow/ice albedo degrades retrievals, improved with version 02.01.03. Occurrence of C(T)H equal to surface height at low cloud fraction, improved with version upgrade. Across track CTH and CF pattern and North-South cloud albedo pattern, improved with version 02.01.03. Cloud fraction: lower dispersion between CLOUD 02.02 and FRESCO 02.02.
		CALv2 CTH (h)	-40%	2 km	
		CALv1 CTH (l)	-15%	0.8 km	
		CALv2 CTH (l)	-15%	0.6 km	
		CRBv1 CH (h)	-20%	1.5 km	
		CRBv2.1 CH (h)	-25%	1.8 km	
L2_AER_AI	NRTI 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. The issue was resolved with the L1B processor upgrade to version 2 in July 2021.
		aerosol index	-1.1 AI unit	0.1 AI unit	
L2_AER_LH	OFFL	aerosol layer height	50 hPa	100 hPa	Over ocean only. Larger bias and dispersion expected over land.

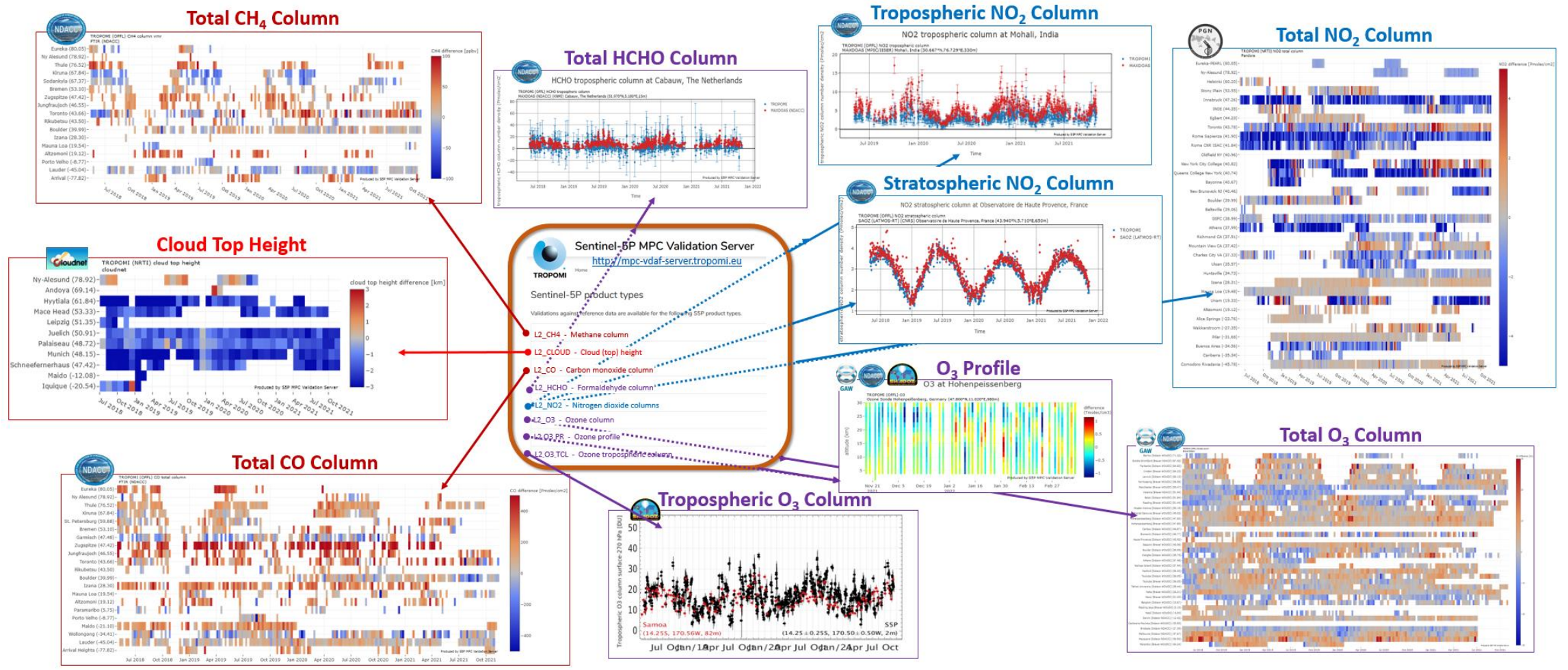
VDAF-AVS: Automated ground-based comparisons and generation of TROPOMI data Quality Indicators



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<https://mpc-vdaf-server.tropomi.eu>

Courtesy, ATM- MPC
BIRA-IASB

FRM PGN operational comparisons



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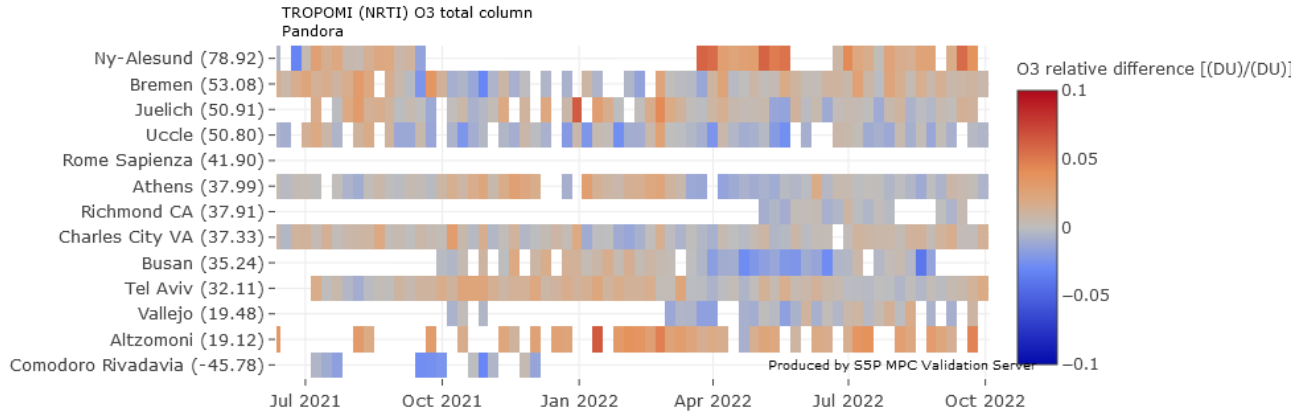


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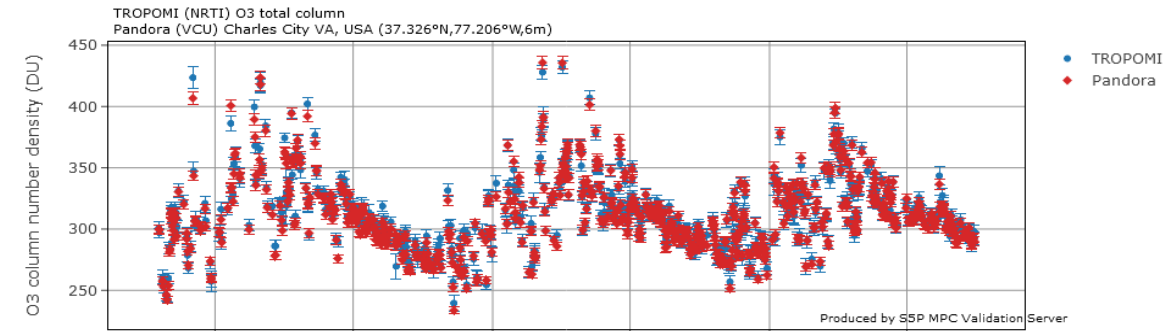


O3 TC comparison (courtesy ATM-MPC)

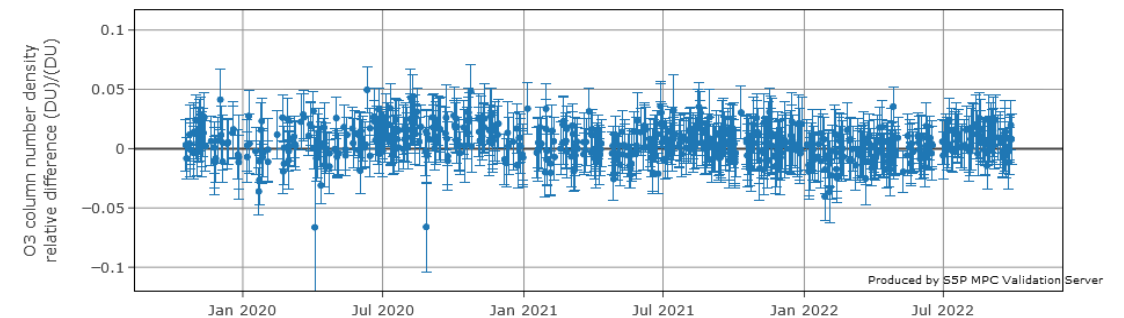
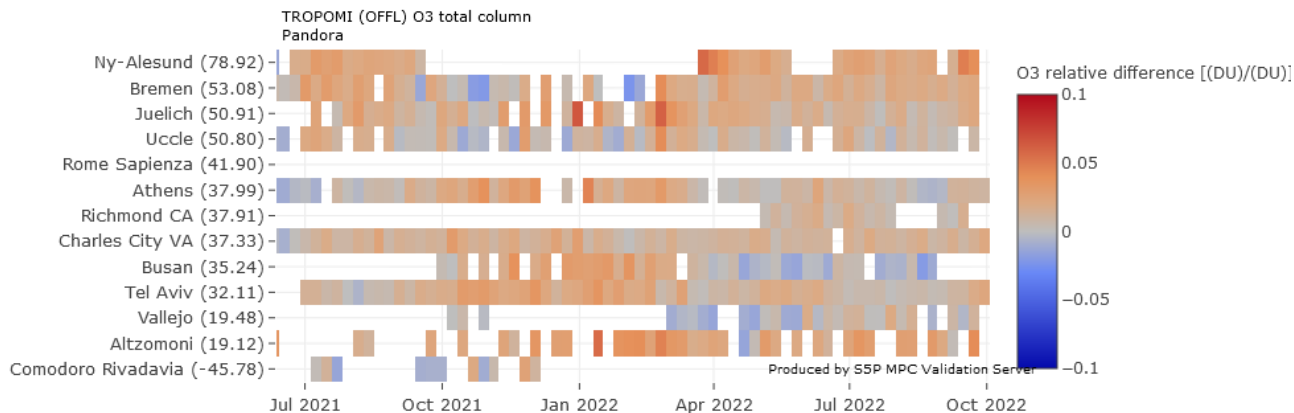
S5P vs PGN: NRTI L2_O3 – relative difference – 13 stations



O3 total column at Charles City VA, USA



S5P vs PGN: OFFL L2_O3 – relative difference – 13 stations

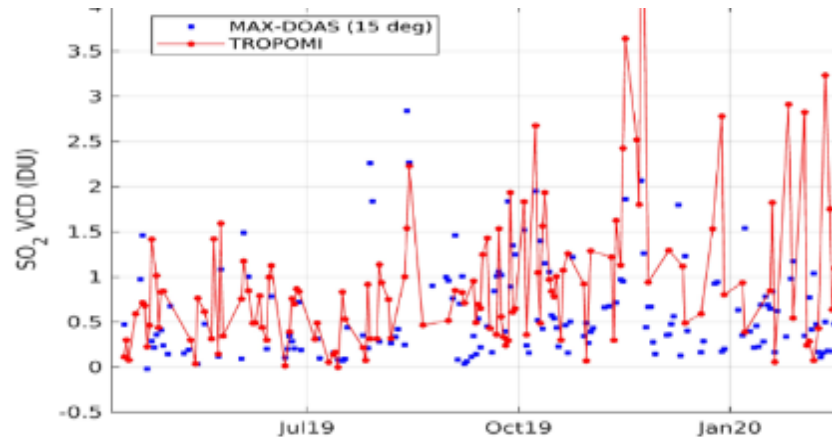
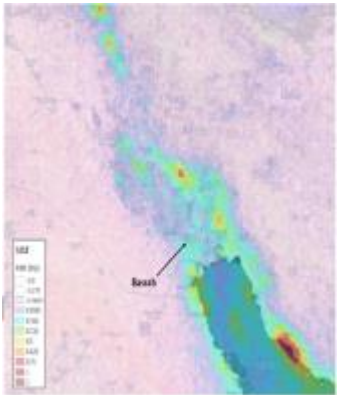


Mean diff: 0.5%
Spread: 1.3%

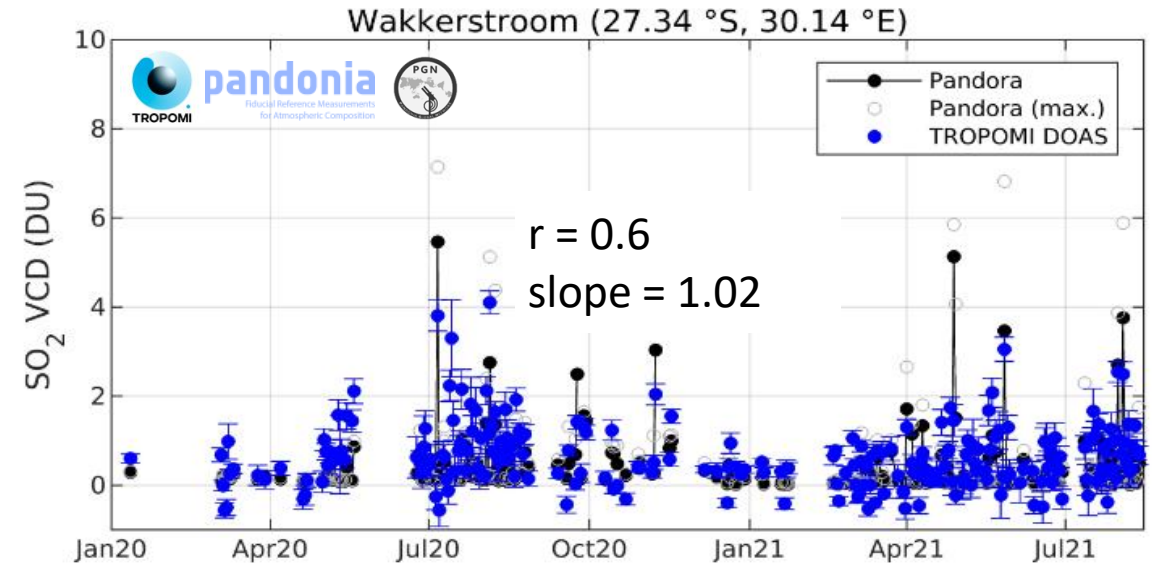
S5P Validation of Sulfur Dioxide Column

- vs. MAX-DOAS : typical bias of 0.2 DU, dispersion 0.2 DU, but larger deviations in winter (NH)
- Good qualitative agreement with GOME-2, OMI, OMPS
- Enhanced validation time series and geographical coverage using PGN/Pandora v1.8 SO₂ measurements

S5P SO₂ vs. MAXDOAS in Basra (Iraq)



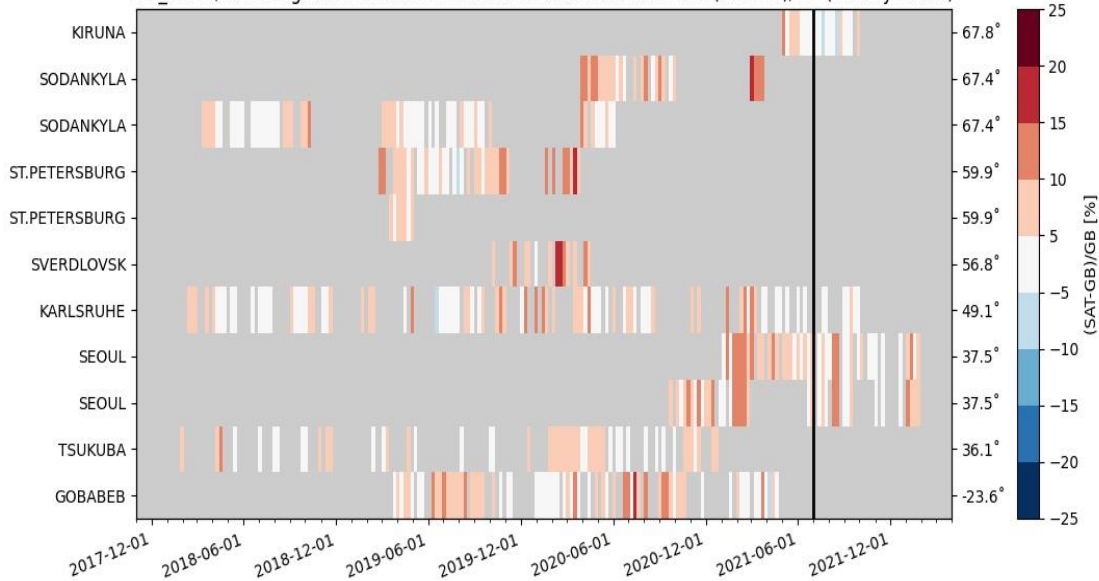
New activity: S5P validation vs. PGN/Pandora



Courtesy, ATM- MPC,
T. Wagner (MPI-C), N. Theys (BIRA-IASB) et al.

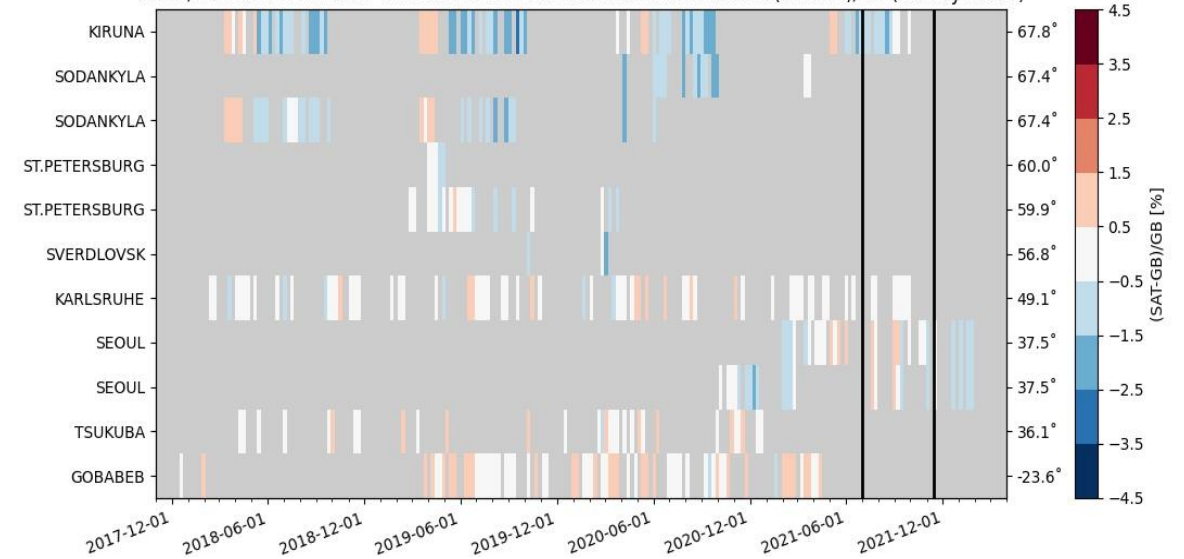
CO and CH₄ comparison (courtesy ATM-MPC)

CO_RPRO/OFFL avg and FTIR.COCCON.CO xCO relative differences (SAT-GB)/GB (weekly mean)



Mean → Bias = 6.08% ; STD = 5.32% ;
correlation coefficient = 0.91

RPRO/OFFL xCH₄ BC and FTIR.COCCON.CH₄ xCH₄ relative differences (SAT-GB)/GB (weekly mean)



Standard XCH₄ Mean → Bias = -0.90% ; STD = 0.78% ; correlation coefficient = 0.59
Bias corrected XCH₄ Mean → Bias = -0.34% ; STD = 0.75% ; correlation coefficient = 0.59



- S5P routine Cal/Val organisation set up since start of mission, monitoring that product mission requirements are met
- Fiducial Reference Measurements for S5P largely set up and operational, examples:
 - Pandora Global Network
 - FRM4DOAS
 - FRM4GHG
 - COCCON