

Sentinel-5p Mission Performance Centre Automated Validation Facility

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Contributions from DLR, IUP-UB, KNMI, MPI-C, NILU, RAL, SRON



Background and Objectives

S5P Mission Performance Centre (MPC) to provide validation service during Copernicus S5P Routine Operation:

- **Automated, routine** comparison of S5P data vs. FRMs
 - Generation of **S5P validation database** for MPC Teams
 - Automated generation of **on-line quick-look reports**
- } machine based
⇒ VDAF
- Validation-based **detection of** L2 products **health issues**
 - Generation of **quarterly** consolidated **validation reports**
 - Validation support to Level-1-to-2 **algorithm QA & evolution**
- } Human ⇒
MPC VAL Team

Background and Objectives

Heritage validation systems at BIRA-IASB



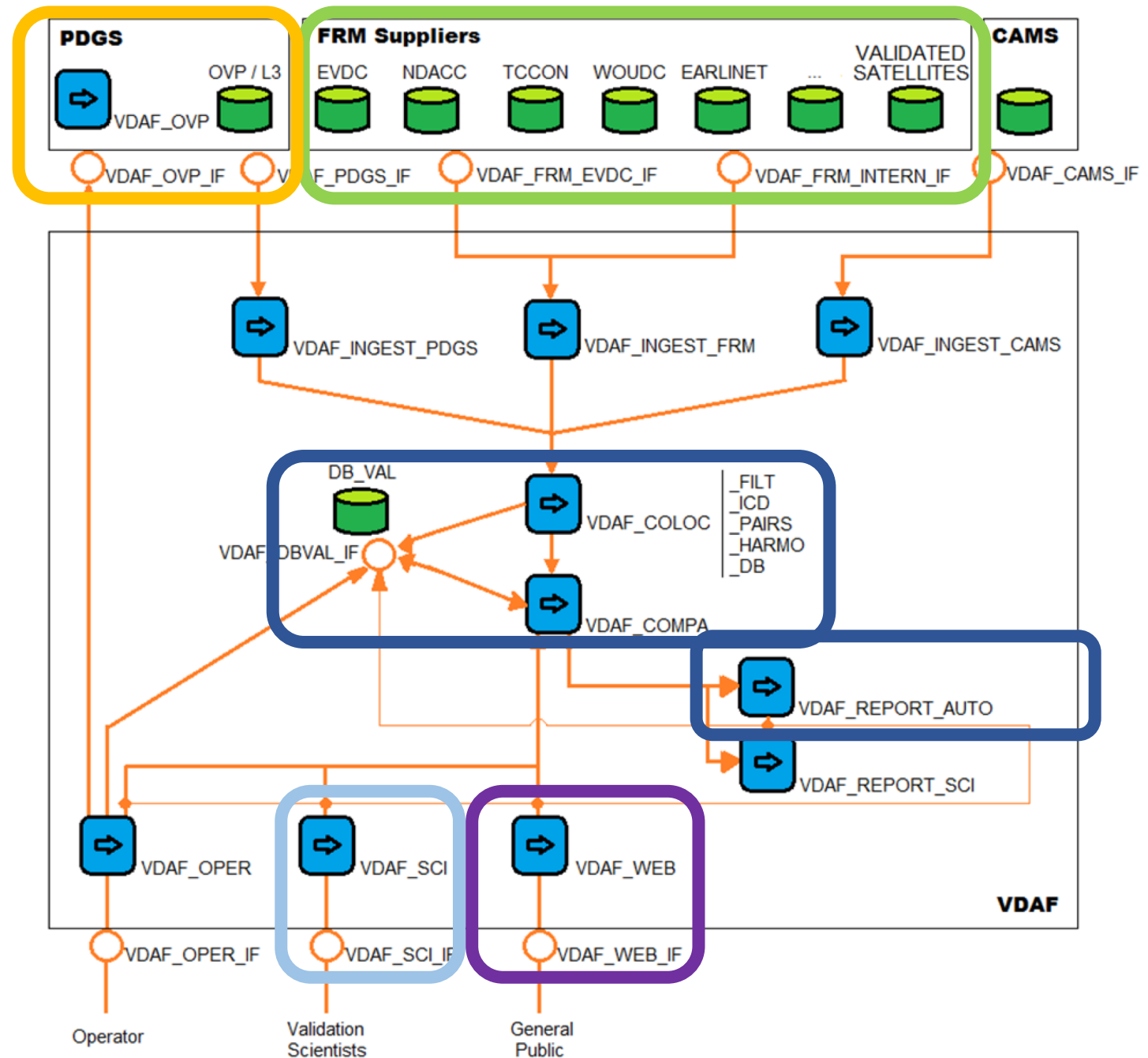
- **Multi-TASTE**: expert validation system for GOME/TOMS/SBUV, Envisat, 14 Limb/Occ... in ACVE, S5PVT, SPARC, WMO/UNEP, CCI_ozone, C3S_312a#4...
- **OSSSMOSE**: Observing System of Systems Simulator (for OSSSEs) with detailed metrology, including error budget closure for data comparisons
- **EUMETSAT AC-SAF**: GOME-2 and IASI trace gas data validation server
- **FP7 NORs**: automated comparison of MACC vs. NDACC
- **CAMS-84/27**: routine evaluation of CAMS vs. NDACC and TCCON
- **FP7 QA4ECV**: ECV QA System + Atmospheric ECVs Validation Server

+s[&t

+ lessons learnt from GSICS, CNRS ICARE, NOAA NPROVS

S5P MPC Validation Data Analysis Facility (VDAF)

System Architecture



State-of-the-Art Validation Chain, Co-locators, Comparators...

Atmos. Meas. Tech., 8, 2093–2120, 2015
 www.atmos-meas-tech.net/8/2093/2015/
 doi:10.5194/amt-8-2093-2015
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Atmospheric Measurement Techniques

Round-robin evaluation of nadir ozone profile retrievals: methodology and results

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

Geoscientific Model Development

Description of algorithms for co-locating and comparing gridded model data with ground-based measurements

Atmos. Meas. Tech., 8, 5039–5062, 2015
 www.atmos-meas-tech.net/8/5039/2015/
 doi:10.5194/amt-8-5039-2015
 © Author(s) 2015. CC Attribution 3.0 License.

Metrology of ground-based satellite validation mismatch and smoothing issues of total ozone

Abstract. Comparisons with ground-based correlative measurements constitute a key component in the validation of satellite data on atmospheric composition. The error budget of these comparisons contains not only the measurement errors but also several terms related to differences in sampling and smoothing of the inhomogeneous and variable atmospheric field. A versatile system for Observing System Simulation Experiments (OSSSE), named OSSSMOSE, is used here to quantify these terms. Based on the application of pragmatic observation operators onto high-resolution atmospheric fields, it allows a simulation of each individual 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 typical case study, the system is used to evaluate the error budget of total ozone column (TOC) comparisons between GOME-type direct fitting (GODFITv3) satellite retrievals

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

Report / Deliverable D2.5

QA4ECV

Assurance for Essential Climate Variables

QA/Validation of Atmospheric ECV Pre-processed Data

Processing

GAIA-CLIM

NPL National Physical Laboratory

Atmos. Meas. Tech. Discuss., 4 August 2015

Received: 23 May 2015 – Published in Atmos. Meas. Tech. Discuss.: 4 August 2015
 Revised: 6 November 2015 – Accepted: 11 November 2015 – Published: 2 December 2015

Abstract. Comparisons with ground-based correlative measurements constitute a key component in the validation of satellite data on atmospheric composition. The error budget of these comparisons contains not only the measurement errors but also several terms related to differences in sampling and smoothing of the inhomogeneous and variable atmospheric field. A versatile system for Observing System Simulation Experiments (OSSSE), named OSSSMOSE, is used here to quantify these terms. Based on the application of pragmatic observation operators onto high-resolution atmospheric fields, it allows a simulation of each individual 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 typical case study, the system is used to evaluate the error budget of total ozone column (TOC) comparisons between GOME-type direct fitting (GODFITv3) satellite retrievals



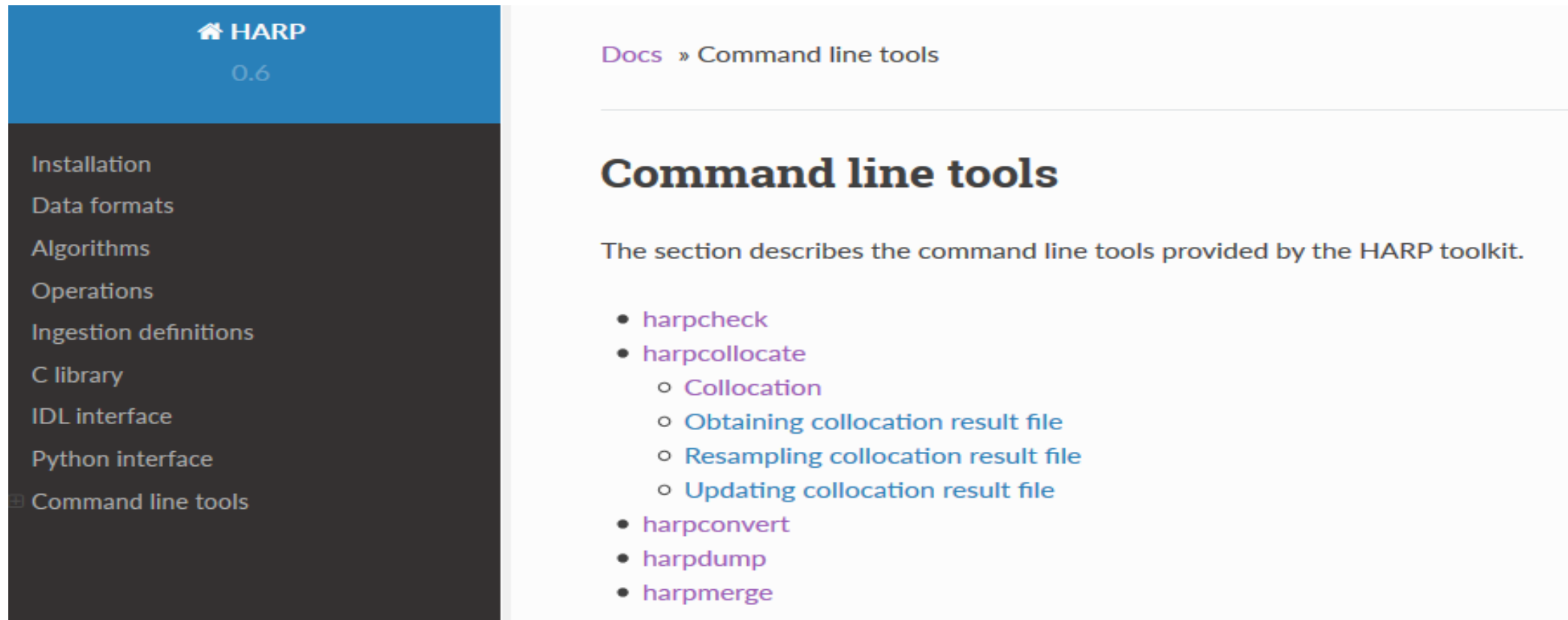
Data Handling, Co-location and Comparison Toolset

HARP



harp documentation

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



The screenshot shows the HARP documentation website. The left sidebar has a blue header with 'HARP 0.6' and a list of navigation items: Installation, Data formats, Algorithms, Operations, Ingestion definitions, C library, IDL interface, Python interface, and Command line tools (which is highlighted). The main content area has a breadcrumb 'Docs » Command line tools' and a heading 'Command line tools'. Below the heading is a paragraph: 'The section describes the command line tools provided by the HARP toolkit.' This is followed by a bulleted list of tools: harpcheck, harpcollocate (with sub-items: Collocation, Obtaining collocation result file, Resampling collocation result file, Updating collocation result file), harpconvert, harpdump, and harpmerge.



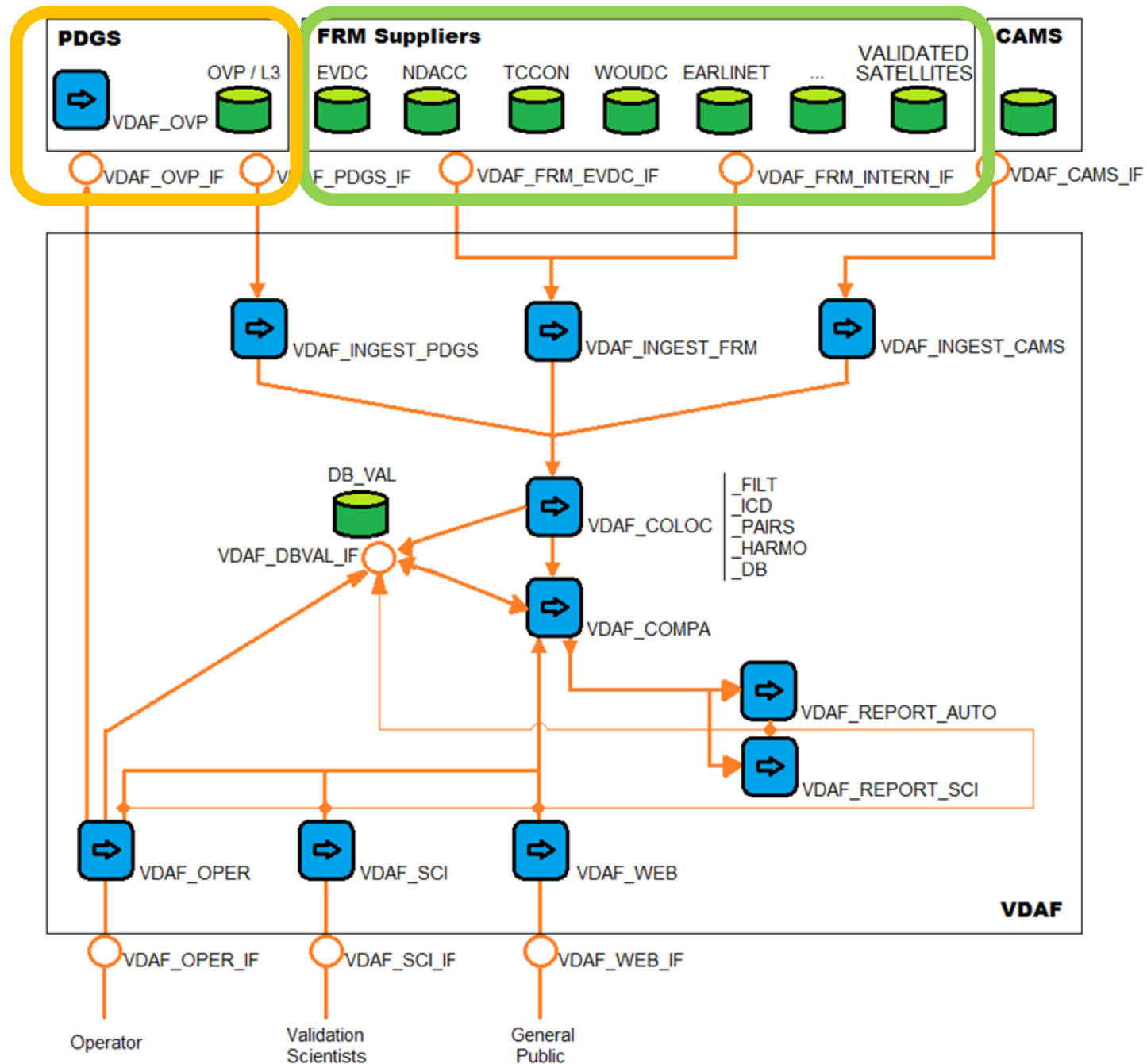
S5P VDAF

S5P TROPOMI

and

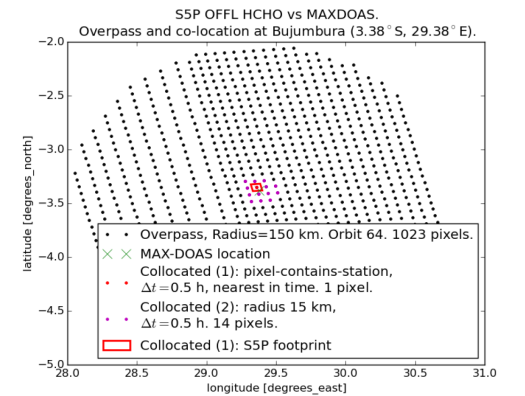
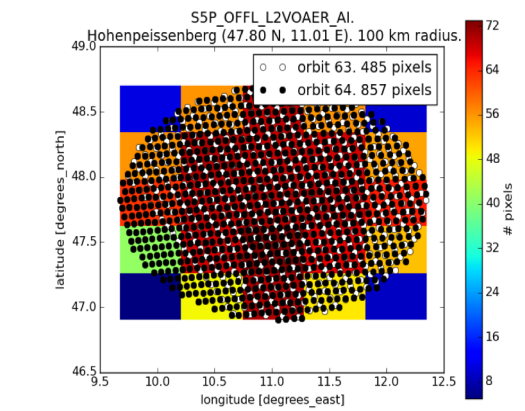
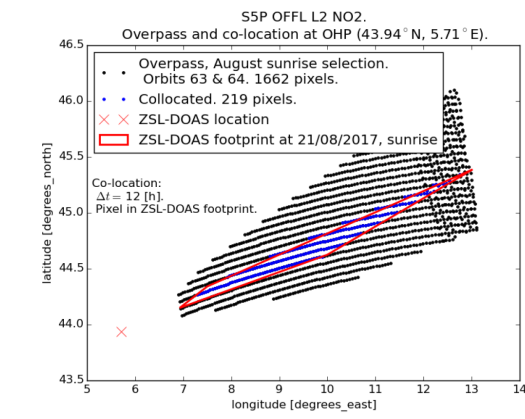
FRM

Data Streams



S5P Data Streams

- Overpass data extractor in S5P PDGS
- Generic approach, specific parameters
- Optimization of data volumes



T. Verhoelst et al.: Co-location mismatch and smoothing issues of total ozone data comparisons AMT 2015

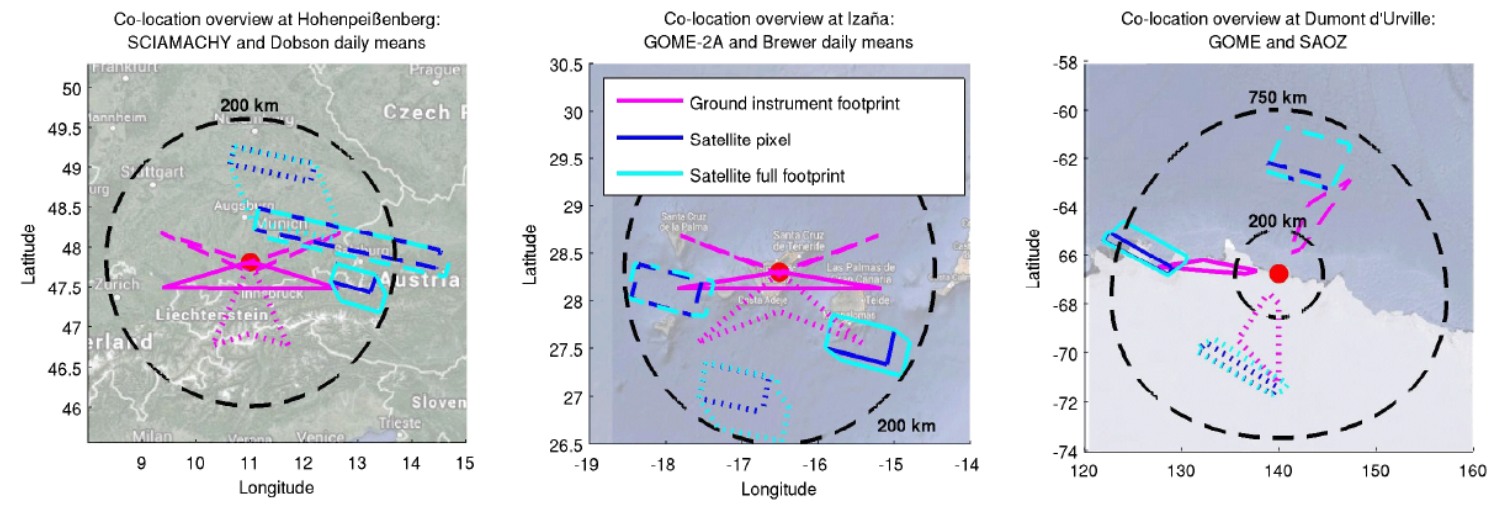


Figure 4. Co-located ground-satellite measurement pairs near summer and winter solstice (dashed and dotted lines, respectively) and near the autumn and spring equinox (solid line). The station is indicated by a red dot, the ground observation operators in magenta, the satellite pixel in dark blue and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

FRM Data Streams into S5P VDAF

ESA FRM programme + WMO GAW contributing networks

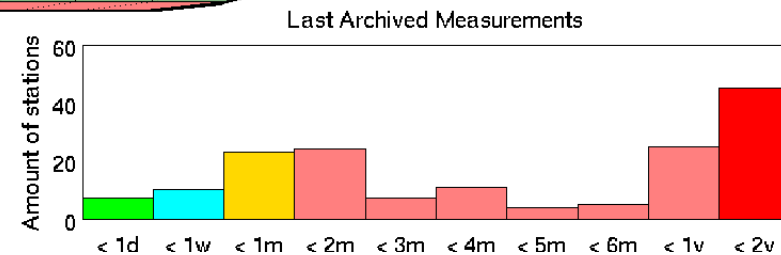
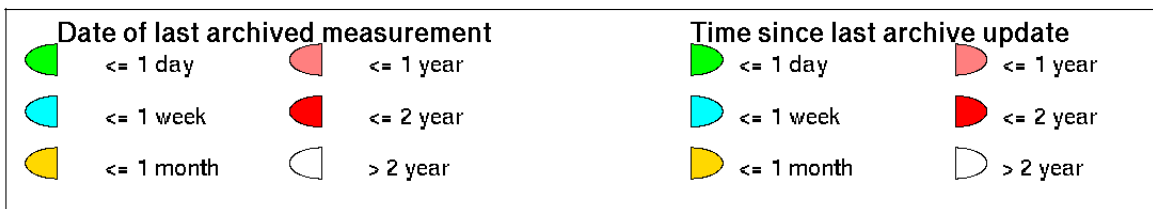
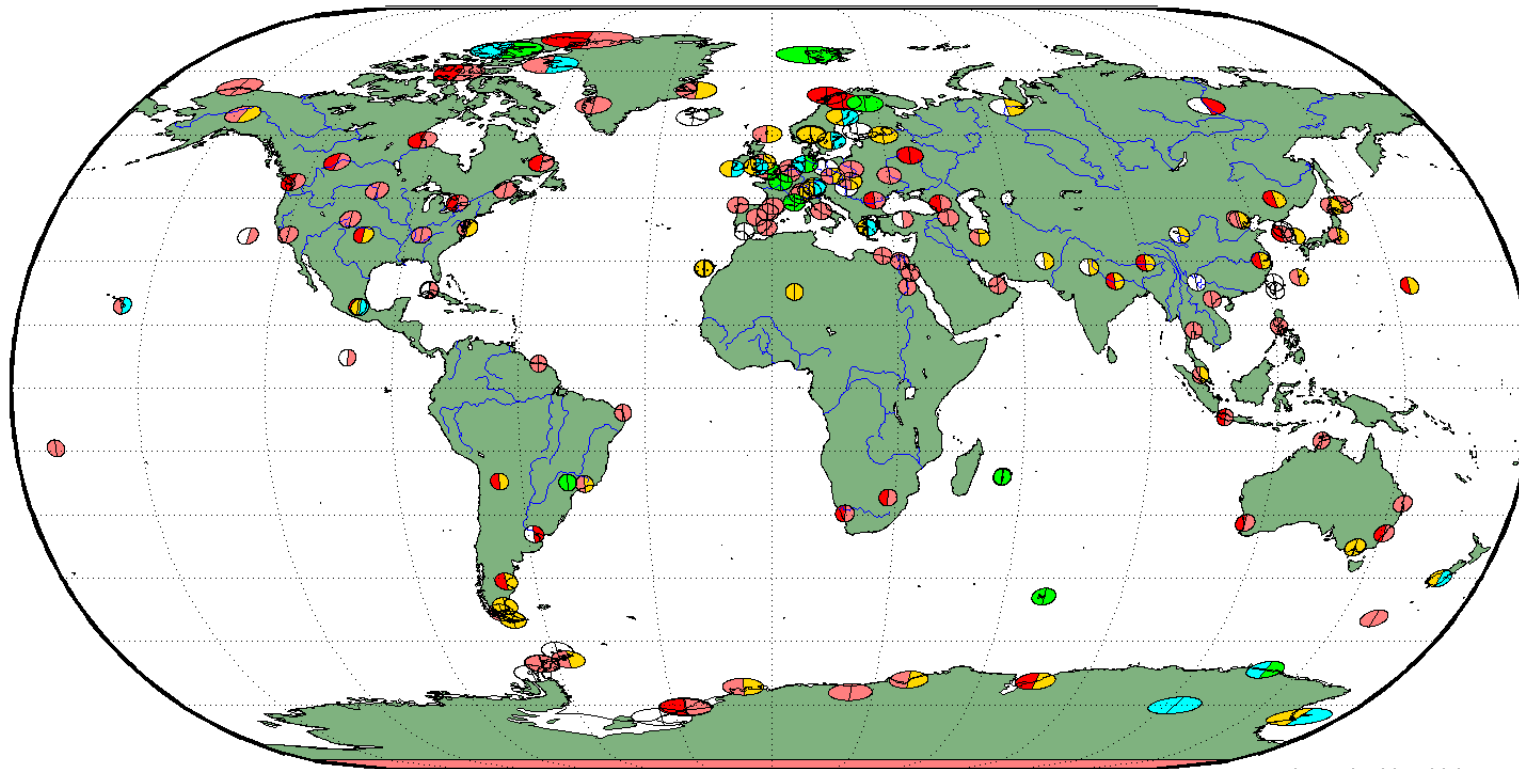


ID	S5P Data Product	Fiducial Reference Measurements
A	O ₃ total column	Brewer, Dobson, ZSL-DOAS, MAX-DOAS, Pandonia
B	O ₃ profile (incl. troposphere)	ozonesonde, stratospheric DIAL, tropospheric DIAL
C	O ₃ tropospheric column	ozonesonde
D	NO ₂ stratospheric column	ZSL-DOAS
	NO ₂ tropospheric column	MAX-DOAS
	NO ₂ total column	Pandonia
E	SO ₂ total column	Pandonia
F	HCHO total column	MAX-DOAS, Pandonia
G	CO total column	TCCON FTIR (NIR), NDACC FTIR (MIR)
H	CH ₄ total column	TCCON FTIR (NIR), NDACC FTIR (MIR)
I	Cloud Fraction	<i>not available</i>
	Cloud Height (pressure)	Cloudnet lidar/radar
	Cloud Optical Thickness	<i>not available</i>
J	Aerosol Absorbing Index	<i>not available</i>
	Aerosol Layer Height	EARLINET aerosol lidar



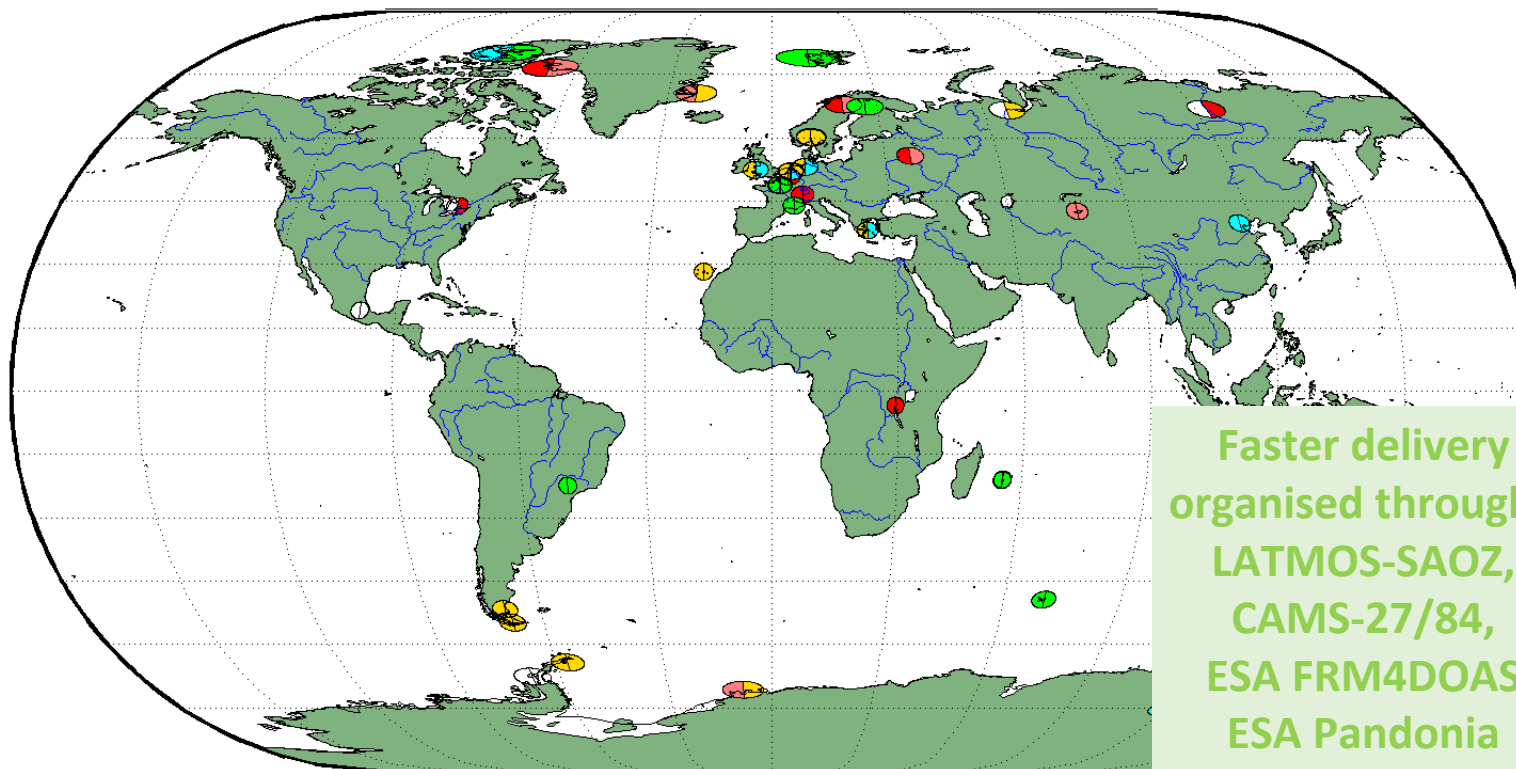
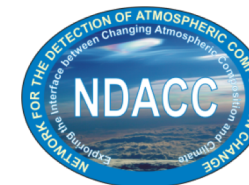
FRM Data Streams into S5P VDAF: O₃ column data

S5P FRM Archiving Rate reportV3_20180412
Ozone Column Network - All archives



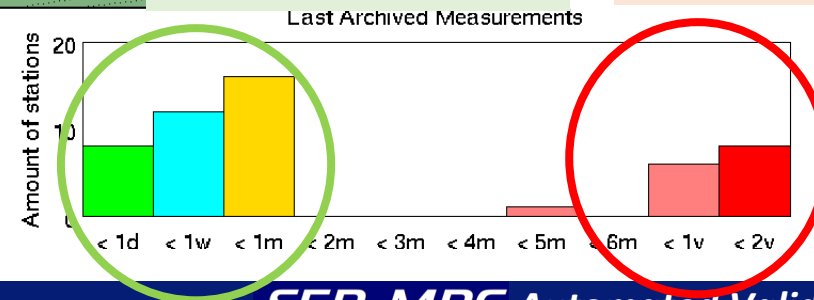
FRM Data Streams into S5P VDAF: Stratospheric NO₂ column data

FRM Archiving Rate report V3_20180412
 NO₂ Column Network - All archives



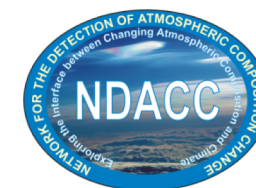
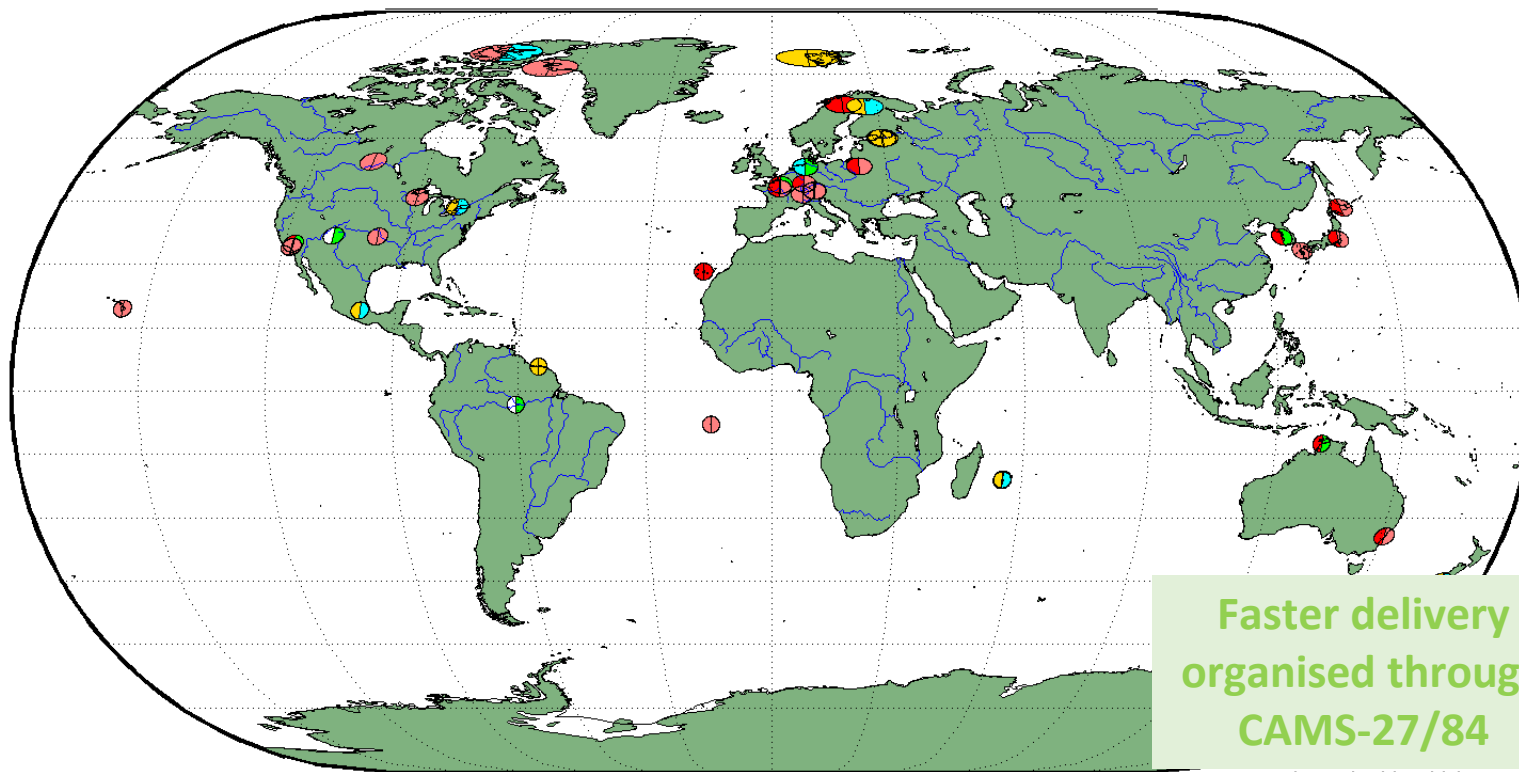
**NDACC
 standard
 archiving rate**

Date of last archived measurement		Time since last archive update	
	<= 1 day		<= 1 day
	<= 1 week		<= 1 week
	<= 1 month		<= 1 month
	<= 2 year		<= 2 year
	> 2 year		> 2 year



FRM Data Streams into S5P VDAF: CH₄ column data

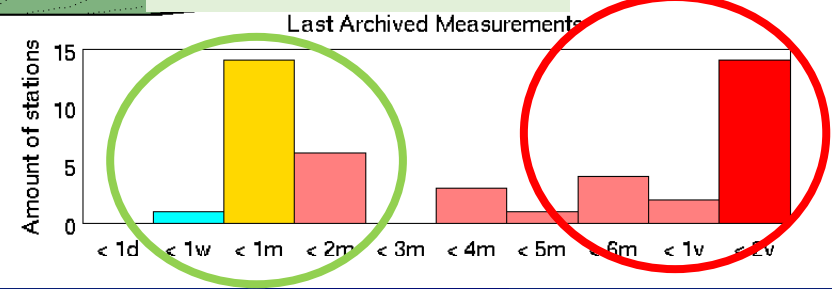
FRM Archiving Rate report v3_20180412
 CH₄ Column Network - All archives



Faster delivery
 organised through
 CAMS-27/84

NDACC & TCCON
 standard
 archiving rate

Date of last archived measurement		Time since last archive update	
	<= 1 day		<= 1 day
	<= 1 week		<= 1 week
	<= 1 month		<= 1 month
	<= 2 year		<= 2 year
	> 2 year		> 2 year

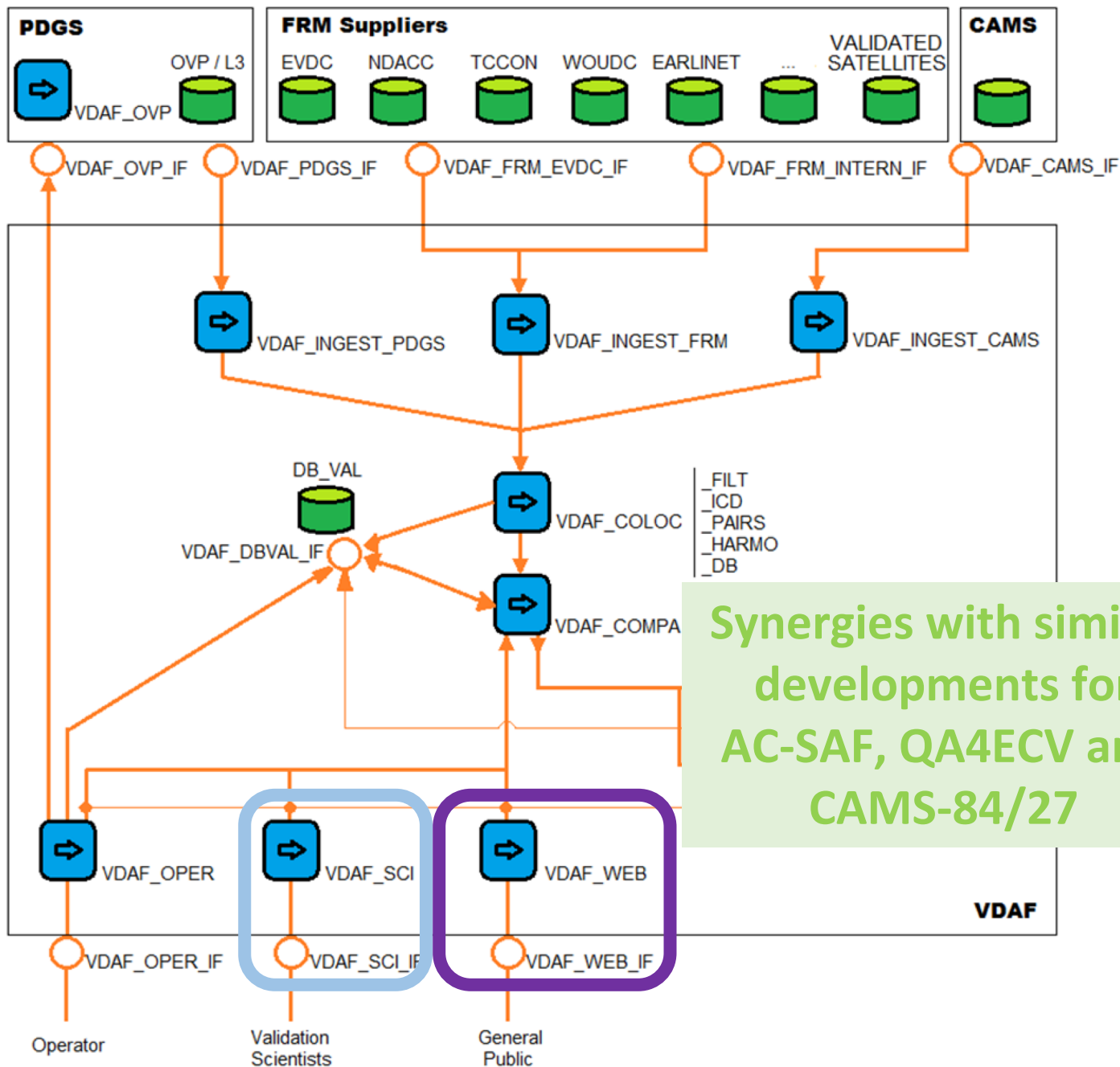


S5P VDAF

MPC dedicated
Automated
Validation
Server

and

Public
Validation
Website



Synergies with similar developments for AC-SAF, QA4ECV and CAMS-84/27

S5P VDAF Automated Validation Server

S5P Validation Server

Home

Step 1: select prod

This is an overview of available product types.

- L2_CH4__ (C
- L2_CO__ (C
- L2_HCHO__ (
- L2_NO2__ (N
- L2_O3__ (O
- L2_O3_PR (C
- L2_O3_TPR (C
- L2_SO2__ (S

S5P Validation

Home / L2_O3__ (O3 total co

Step 3: select

- Bauru (ZSL-DOAS latmos_rt)
- Dumont d'Urville (ZSL-DOAS lat
- Guyancourt (ZSL-DOAS latmos
- Kerguelen (ZSL-DOAS latmos
- OHP (ZSL-DOAS latmos_rt)
- Paris (ZSL-DOAS latmos_rt)
- St. Denis (ZSL-DOAS latmos_rt)

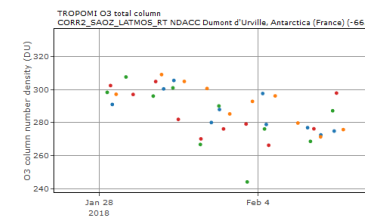
S5P Validation Server

Home / L2_O3__ (O3 total column) / O3 total column OFFL vs ZSL-DOAS - / Dumont d'Urville (ZSL-DOAS latmos_rt) -

O₃ total column | CORR2_SAOZ_LATMOS_RT NDACC at Dumont d'Urville, Antarctica (France)

Averaged Properties

Averaged



	TROPOMI (sunrise area)	CORR2_S
Mean	295.38 DU	296.80 DU
SEM	2.9172 DU	2.8022 DU
Std. dev.	15.978 DU	15.348 DU
RMS	295.80 DU	299.18 DU
Median	298.80 DU	299.00 DU
IGR	24.451 DU	24.236 DU
Count	30	30

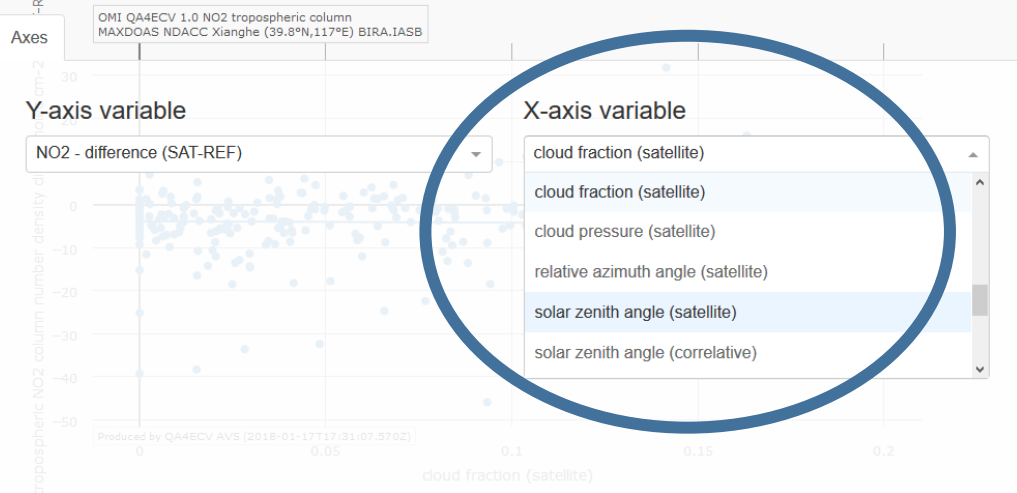
Settings

Correlative plot

compare miscellaneous quantities

Settings

Correlative plot at Xianghe



S5P Validation Server

Home / O3 total column / latmos_rt at Dumont d'Urville

O₃ total column | CORR2_SAOZ_LATMOS_RT NDACC at Dumont d'Urville, Antarctica (France)

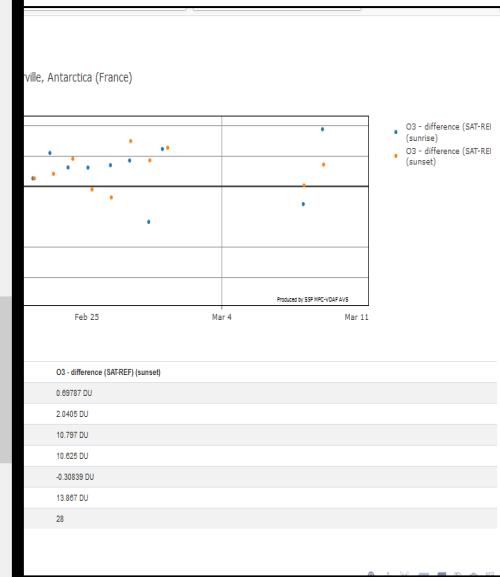
Averaged Properties

Properties

Processing traceability

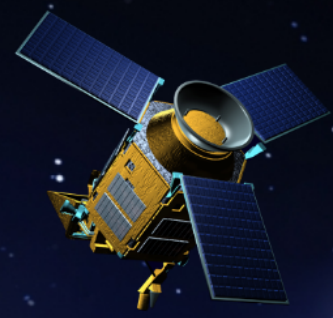
Download Harp commands in yami format:

- averaged sunrise
- averaged sunset





<http://tropomi.eu> => <http://s5p-mpc-vdaf.aeronomie.be>



SENTINEL 5P

MISSION PERFORMANCE CENTER VALIDATION FACILITY

- Ozone
- O3 profile
- Nitrogen dioxide
- Sulfur Dioxide
- Formaldehyde
- Surface UV-B
- Aerosols
- Carbon Monoxide
- Methane
- Cloud

TROPOMI
TROPOspheric Monitoring Instrument

SCIENCE WEBSITE
[VIEW S5P/TROPOMI WEBSITE](#)



S5P MPC Validation Website

Home For researchers Search Browse by

TROPOMI

SENTINEL 5P

MISSION PERFORMANCE CENTER
VALIDATION FACILITY

Ozone O3 profile Nitrogen dioxide Sulfur Dioxide Formaldehyde

Surface UV-B Aerosols Carbon Monoxide Methane Cloud

Home For researchers Search Browse by Target Contact us

Ozone
Ozone profile
Formaldehyde
Methane
Carbon Monoxide
Aerosol
Nitrogen Dioxide
Sulphur Dioxide

Ozone column

Tropomi provides O₃ column data products:
[Total Ozone column](#)
[Tropospheric Ozone column](#)

This page shows the most recent validation reports.

O3 total column at Hohenpeißenberg, Germany

TROPOMI O3 total column
CORR2_NDACC BREWER NDACC Hohenpeißenberg, Germany (47.800°N, 11.020°E, 980m)

O3 column number density (DU)

Time

Produced by SSP MPC-VDAF AVS

Settings

Preliminary data and results! - S5P in Commissioning Phase...

S5P MPC Validation Website

Dr. Bavo Langerock (baval@oma.be)

Period	2018-01-23 - 2018-03-21
Successful reports/Total Reports	508/1505: 34%
Failed Quality Assurance checks/Total Reports	342/1505: 23%
Failed Rapid Delivery checks/Total Reports	878/1505: 58%

Filters:

SUBMISSION DATE	PRODUCT ID	FILENAME	RD	QA	REPORT
2018-03-21	ftir.o3_spbu001	groundbased_ftir.o3_spbu001_st.petersburg_201801231112931z_201802271135219z_001.hdf	🔴	🟢	📄
2018-03-21	lidar.o3_nasa_jpl002	groundbased_lidar.o3_nasa_jpl002_mauna.loa.hi_201803071064958z_201803071094641z_001.hdf	🟢	🟢	📄
2018-03-21	lidar.o3_nasa_jpl002	groundbased_lidar.o3_nasa_jpl002_mauna.loa.hi_201803081061138z_201803081081205z_001.hdf	🟢	🟢	📄
2018-03-21	lidar.o3_nasa_jpl002	groundbased_lidar.o3_nasa_jpl002_mauna.loa.hi_201803111064443z_201803111083831z_001.hdf	🟢	🟢	📄
2018-03-21	lidar.o3_nasa_jpl002	groundbased_lidar.o3_nasa_jpl002_mauna.loa.hi_201803151060700z_201803151072254z_001.hdf	🟢	🟢	📄
2018-03-21	lidar.o3_nasa_jpl002	groundbased_lidar.o3_nasa_jpl002_mauna.loa.hi_201803171071336z_201803171092016z_001.hdf	🟢	🟢	📄
2018-03-21	lidar.o3_nasa_jpl002	groundbased_lidar.o3_nasa_jpl002_mauna.loa.hi_201803181063001z_201803181083714z_001.hdf	🟢	🟢	📄
2018-03-21	lidar.o3_nasa_jpl002	groundbased_lidar.o3_nasa_jpl002_mauna.loa.hi_201803191064254z_201803191084610z_001.hdf	🟢	🟢	📄
2018-03-21	mwr.o3_iup001	groundbased_mwr.o3_iup001_ny.alesund_201803181000705z_201803181210458z_004.hdf	🟢	🟢	📄
2018-03-21	mwr.o3_ubern001	groundbased_mwr.o3_ubern001_bern_201803041000019z_201803041235937z_009.hdf	🟢	🟢	📄
2018-03-21	mwr.o3_ubern001	groundbased_mwr.o3_ubern001_bern_201803051000001z_201803051235948z_009.hdf	🟢	🟢	📄
2018-03-21	mwr.o3_ubern001	groundbased_mwr.o3_ubern001_bern_201803061000017z_201803061235951z_009.hdf	🟢	🟢	📄
2018-03-21	mwr.o3_ubern001	groundbased_mwr.o3_ubern001_bern_201803071000016z_201803071235945z_009.hdf	🟢	🟢	📄
2018-03-21	mwr.o3_ubern001	groundbased_mwr.o3_ubern001_bern_201803081000008z_201803081235621z_009.hdf	🟢	🟢	📄

Many synergies with similar developments for CAMS-27

BIRA-IASB SQL database tailored to CAMS-27, now being ported to S5P MPC VDAF

Conclusion (1/2)

- S5P VDAF Automated Validation Server builds on integration of heritage state-of-the-art satellite/CAMS validation systems (long-term support from BELSPO, EC, ESA, EUMETSAT, ECMWF)
- VDAF-AVS = core of S5P MPC routine validation service
 - implemented in MPC environment
 - tailored to Copernicus and S5P needs
 - developed in synergy with other Copernicus elements
- Starting soon routine validation service for S5P trace gas data, with continuous verification of L2 health and quarterly validation reporting



Conclusion (2/2)

- VDAF/HARP tools expandable virtually to all atmospheric species, and possibly to other domains and applications
- Valuable synergies/convergence between Copernicus space, (FRM) data procurement and service components
- Enhanced coordination desired for approach to/funding for FRM gap analysis, deployment, data generation and delivery
- Support needed for operationalization of scientific systems, service set-up, improvement of tools and methods, harmonization of uncertainty expression, implementation of comparison error budget closure...
- Automated or not, EO (L1/L2/L3/L4) data validation always requires substantial interpretation by (human) scientific experts !



Thank you !