# Sentinel-5 Precursor Mission and Cal/Val lessons learned

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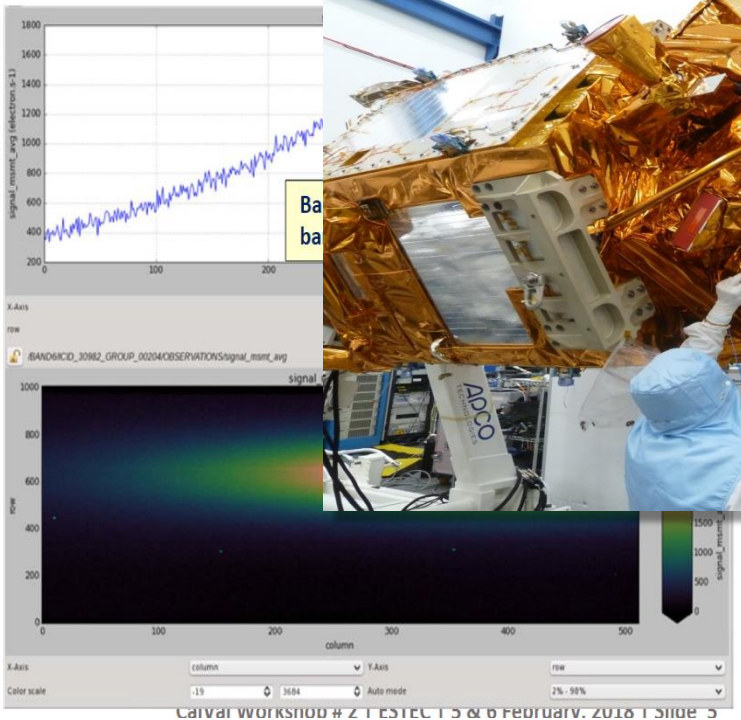
# Importance of the pre-flight calibration campaign!

- 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**

# 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**

# Cal/Val Organisation for the Sentinels

***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.*

## The Sentinel Validation Teams (SVT):

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

***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)*

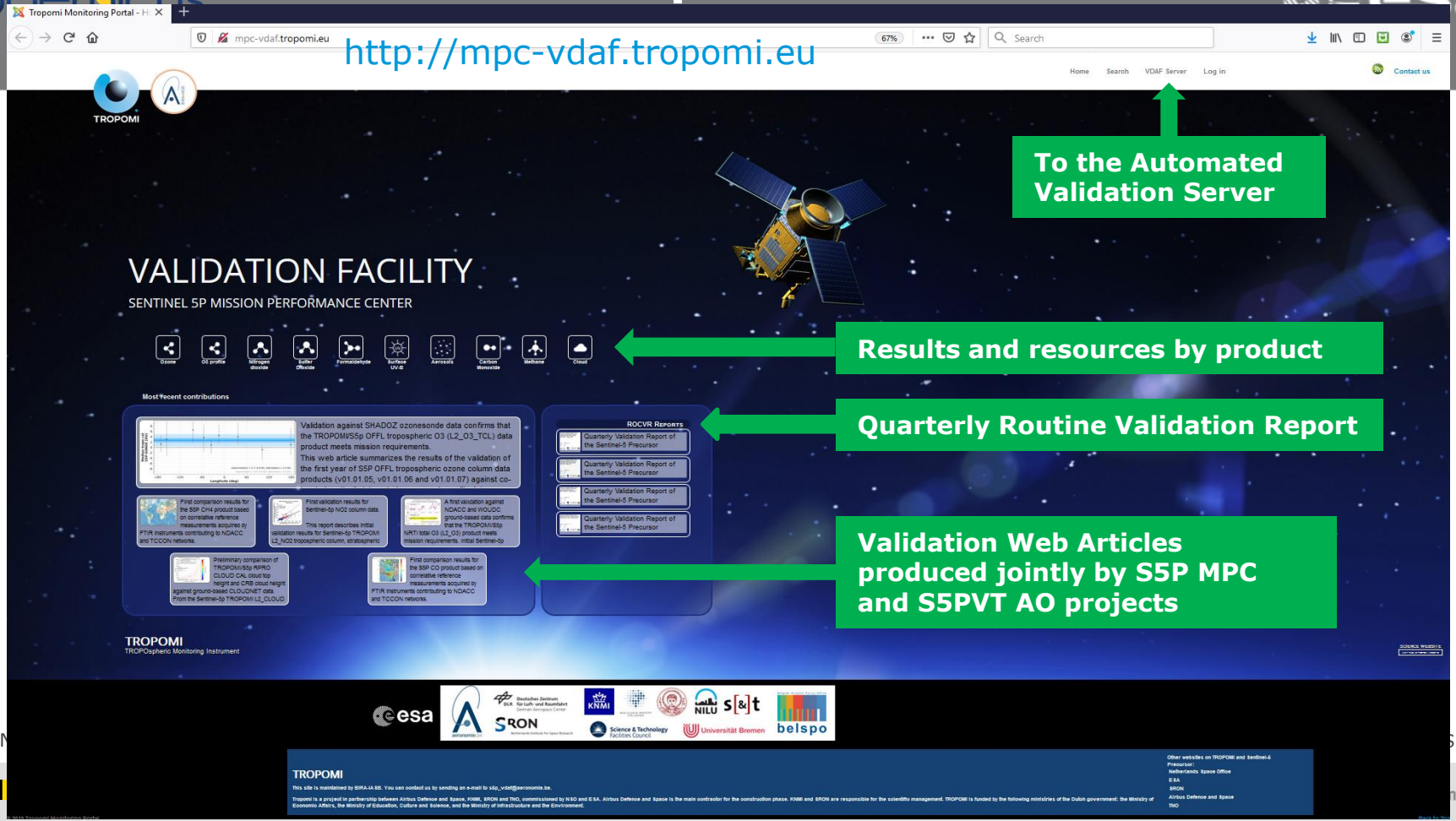
## User Community and international forum:

*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***

# MPC Routine Operations Validation

http://mpc-vdaf.tropomi.eu



# S5P MPC Quality Information Output



## 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 snow/ice 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<br>$NO_2$ stratosphere<br>$NO_2$ total | -22%<br>-9%<br>0±50% | 3.6 Pmol/cm$^2$<br>0.4 Pmol/cm$^2$<br>- | Total $NO_2$ bias depending on total column: pristine areas to slight pollution overestimated, high pollution underestimated. |
| | OFFL RPRO | $NO_2$ troposphere<br>$NO_2$ stratosphere<br>$NO_2$ total | -23%<br>-6%<br>0±50% | 3.6 Pmol/cm$^2$<br>0.3 Pmol/cm$^2$<br>- | |
| L2_HCHO | NRTI OFFL RPRO | HCHO low<br>HCHO high | +26%<br>-31% | 7 Pmol/cm²<br>13 Pmol/cm$^2$ | Positive bias over clean areas (<2 Pmol/cm²), negative bias over large emissions (> 8 Pmol/cm²). |
| 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<br>CRB CH<br>CAL COT | -20%<br>-30%<br>+7.9 [-] | 2 km<br>1 km<br>- | Bias towards the a priori cloud height up to and including 01.01.07. Snow/ice degrades retrievals. Occurrence of C(T)H 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<br>CRB CH<br>CAL COT | -20%<br>-30%<br>+7.9 [-] | 2 km<br>1 km<br>- | |
| L2_AER_AI | NRTI | 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 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. |

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.

S5P MPC

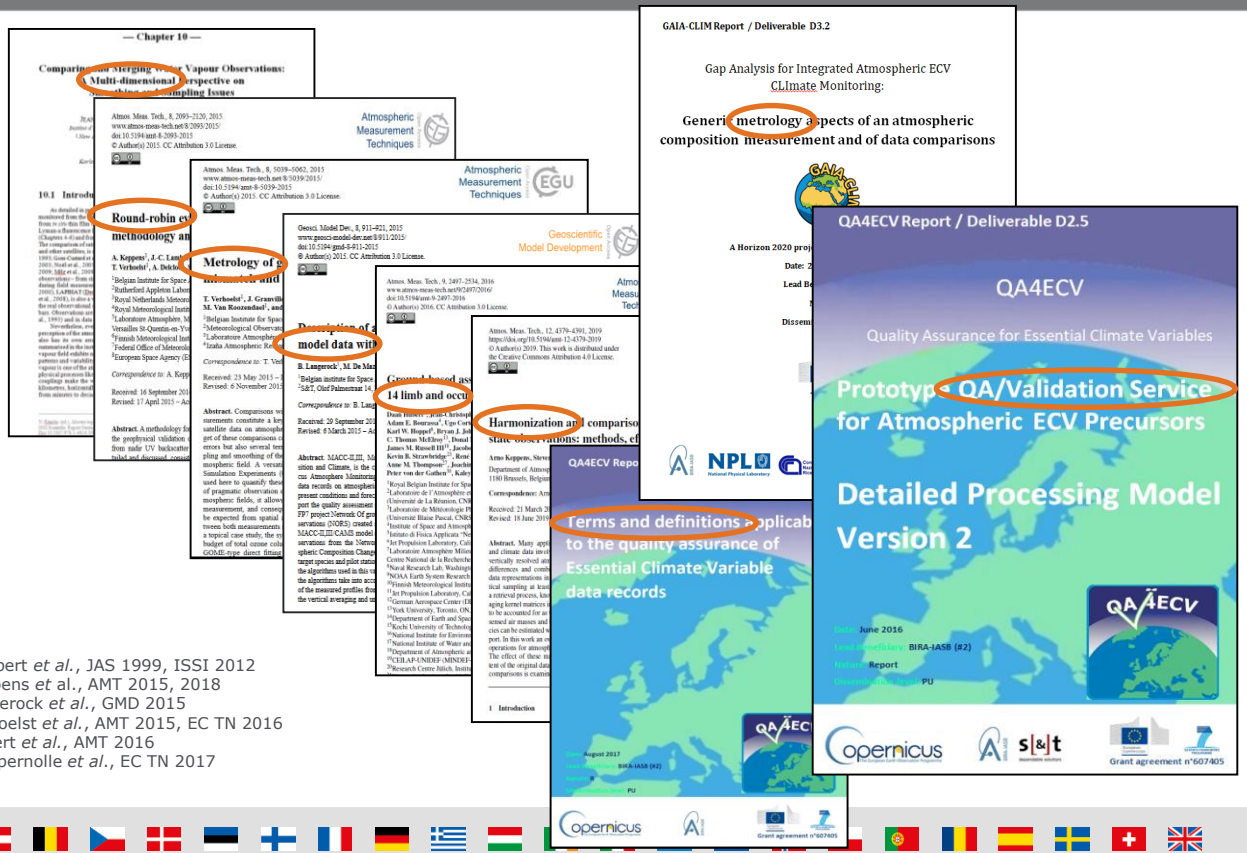

# Validation Data Streams into S5P MPC

## 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 | *not available (satellite-to-satellite only)* |
| | Cloud Height (pressure) | **Cloudnet lidar/radar**, ARM |
| | Cloud Optical Thickness | *not available (satellite-to-satellite only)* |
| L2_AER | UV Aerosol Absorbing Index | *not available (satellite-to-satellite only)* |
| | 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




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
Compernolle *et al.*, EC TN 2017

GEO CEOS QA4EO
WGCV-28/…/31

Cross GEOSS/ cross-EO domains Cal/Val harmonization

esa cci ozone

Prototyping in Multi-TASTE and ESA CCI_Ozone

CEOS
AC(V)C-8/…/11

Community feedback & endorsement

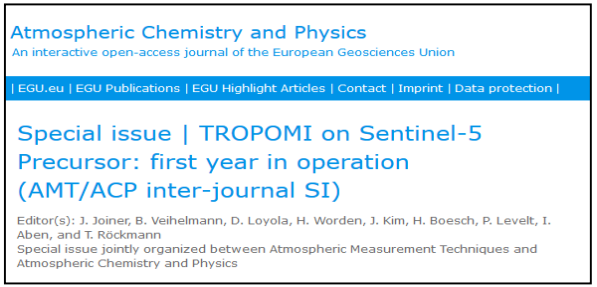
TROPOMI
Climate Change Service

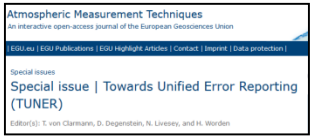
Implementation and continuous development in FP7 QA4ECV, H2020 GAIA-CLIM, Envisat QWGs, ISSI Cross-EO Val., CCI+/C3S ozone, **Sentinel-5p MPC**

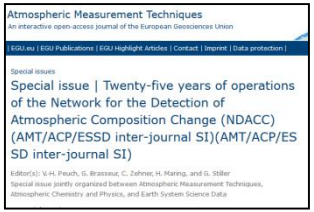
# Generic validation chain, state-of-the-art co-locators, harmonised terminology and comparison metrics… in permanent evolution

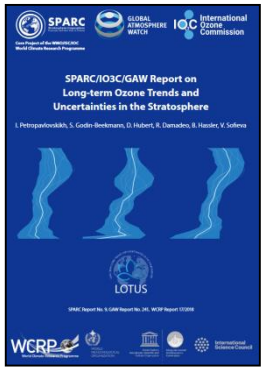
## S5P TROPOMI validation and FRM programme contribute further progress in:

- 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





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Langerock *et al.*, GMD 2015
Verhoelst *et al.*, AMT 2015, EC TN 2016, **AMT 2020**
Hubert *et al.*, AMT 2016, **LOTUS 2019**, **AMT 2020**
Compernolle *et al.*, EC TN 2017, **ACP 2019**, **AMT 2020**
Vigouroux *et al.*, **AMT 2020**

# Sentinel-5p Lessons Learnt
## about data

### 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

# Sentinel-5p Lessons Learnt
## about methods and tools

### 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

# Sentinel-5p Lessons Learnt
## and validation needs for the Air Quality Constellation

### Recommendations

1. 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.
2. Conduct joint validation campaigns with exchange of reference airborne and ground-based instruments.
3. 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.
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.
5. Systematically process the Level-2 Constellation Products of the Geo-AQ missions, using one selected common algorithm per Constellation Product.
6. 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.
7. 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.
8. 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