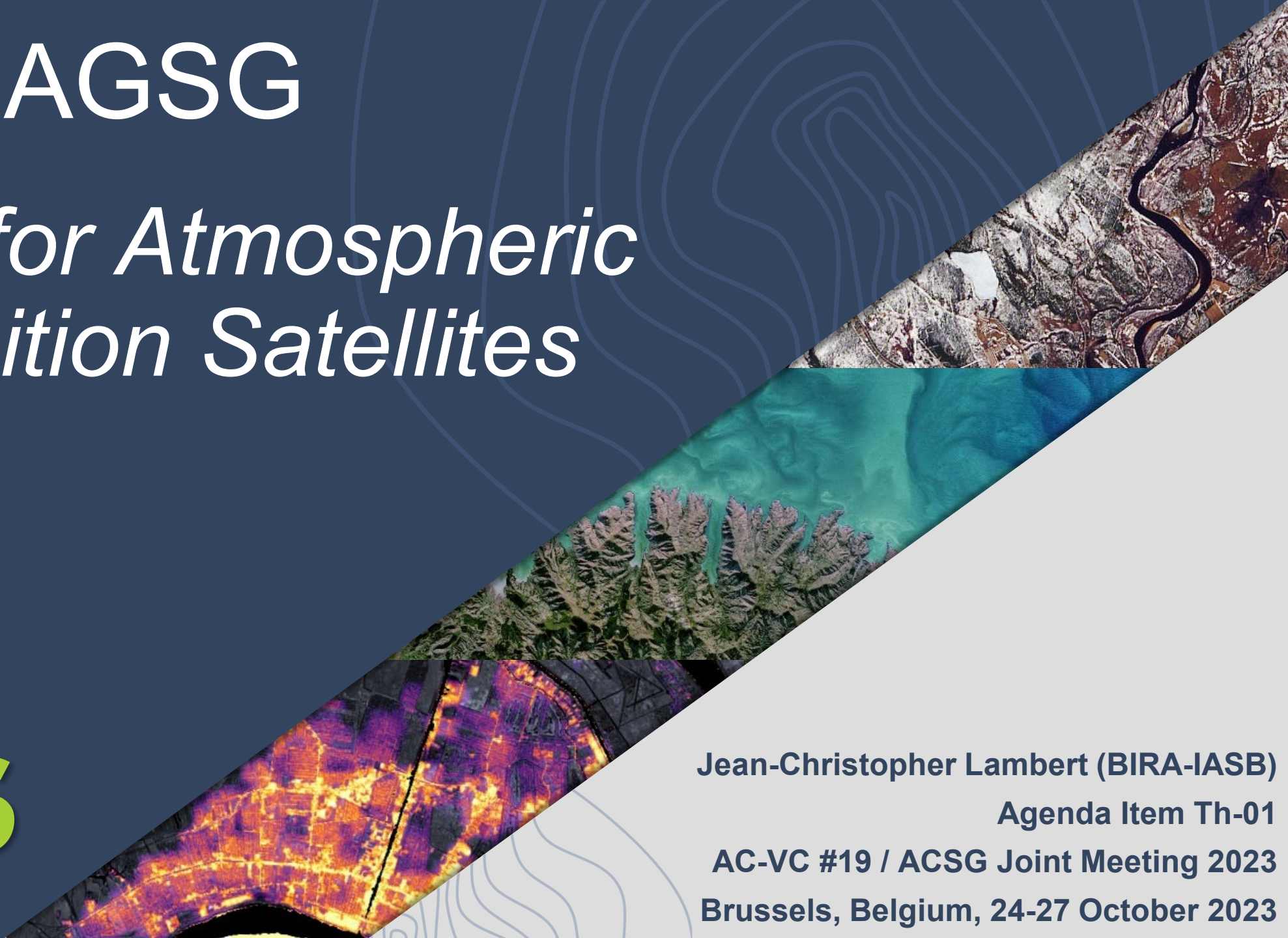
WGCV AGSG

Cal/Val for Atmospheric Composition Satellites



CEOS
Committee on
Earth Observation Satellites

Jean-Christopher Lambert (BIRA-IASB)

Agenda Item Th-01

AC-VC #19 / ACSG Joint Meeting 2023

Brussels, Belgium, 24-27 October 2023

Cal/Val for Atmospheric Composition

1. WGCV & ACSG
2. Highlights on recent activities
3. Cal/Val for the Constellations

WGCV ACSG

Working Group on Calibration and Validation (WGCV) *(talk Th-10 by A. Kuze)*

Several AO domains, Atmospheric Composition SG since 2001 *(this talk)*

WGCV activities with relevance to atmospheric composition missions

- Pre-flight/in-flight calibration, SI-Traceable Satellites *(talks Th-04, Th-07, Th-08)*
- Cal/Val best practices and protocols *(e.g., talk Th-05 by R. Koopman)*
- Support to Cal/Val networks: RadCalNet, HYPERNETS, TIRCALNET, FRM tailoring and infrastructures… *(e.g., talk Th-06 by A. Dehn)*
- FRM Maturity Assessment Framework *(talk Th-02 by N. Fox)*
- CEOS Cal/Val Portal *(talk Th-03 by P. Castracane)*
- CEOS-ARD certification, VH-RODA, New Space…
- Interoperability framework: vocabulary, architecture, interfacing, quality, policy
- Collaboration with WMO, ISO/OGC, IMEO, CGMS-GSICS *(talk Th-09 by L. Flynn)*

L1B Calibration and Validation

- Best practices: vicarious, DCC, PICS, SNO, Rayleigh Scattering, GEO/LEO, […] and SITSat
- SWIR Cal/Val for GOSAT-1/2, OCO-2/3 & TROPOMI
  (see Tu-21 talk by S. Kei and Th-10 talk by A. Kuze)
  - Regular OCO-GOSAT-TROPOMI Calibration Meetings
  - RRV campaigns website at JAXA https://www.eorc.jaxa.jp/GOSAT/GHGs_Vical/index.html
- Collaboration with CGMS-GSICS *(see Th-09 talk by L. Flynn)*
  - UVN Spectrometer Break Out Session at GSICS annual meeting 2023/03
  - Pre-flight optical sensors calibration workshop, ESA/ESTEC, 2024/11
- SI-Traceable Satellites (SITSat) *(see Th-04 talk by M. Thankappan)*

UVN Spectrometer Break Out Session		
Chair: Larry Flynn: Minutes:		
Time	**Title**	**Presenter**
13:30	CMA OMS pre-launch calibration & instrument performance	Yuan Li, CMA (Remote)
13:45	TropoMI Calibration	Melanie Coldewey-Egbers, DLR (Remote)
14:00	Changes in observed straylight in TROPOMI	Antje Ludewig, KNMI (Remote)
14:15	GOME-2 End of Life tests	Alessandra Cacciari, EUMETSAT (Remote)
14:30	ESA FDR4ATMOS project	Melanie Coldewey-Egbers DLR (Remote)
14:45	OMPS Calibration	Banghua Yan, NOAA
15:00	GEMS Calibration and Solar	Mijin Eo, EWHA
15:15	EPIC Calibration	Jay Herman (Remote)
15:30	Break	
15:45	TEMPO Calibration	Xiong Liu, CFA (Remote)
16:00	OMI and TropoMI V2 solar records	Sergey Marchenko, SSAI/NASA
16:15	Inter-calibration approaches for GEMS	Yeeun Lee, EWHA
16:30	OCO-3/GEMS XCO2 and NO2 Near-Simultaneous Observations	Thomas Kurosu, NASA/JPL (Remote)
16:45	V8TOz as a transfer standard	Larry Flynn, NOAA

CEOS-FRM Assessment Framework

Roadmap towards an Assessment Framework for Fiducial Reference Measurements (FRM)

Th-02 talk by Nigel Fox

Just published on https://calvalportal.ceos.org/web/guest/frms-assessment-framework

Next step: pilot applications, ESA FRM4DOAS project for Atmospheric Composition

Self-assessment					Independent assessor
Nature of FRM	FRM Instrumentation	Operations/ sampling	Data	Metrology	Verification
Descriptor	Instrument Documentation	Automation level	Data completeness	Uncertainty Characterisation	Guidelines adherence
Location/ availability of FRM	Evidence of traceable calibration	Measurand sampling	Availability and Usability	Traceability Documentation	Utilisation/Feedback
Range of sensors	Maintenance plan	ATBDs on processing/software	Data Format	Comparison/calibration of FRM	Metrology verification
Complementary observations	Operator expertise	Guidelines on transformation to satellite Pixel	Ancillary Data	Adequacy for intended class of sensors	Independent Verificaton
				FRM CLASSIFICATION	**A B C D** (to be selected)

Grade
Not Assessed
Not Assessable
Basic
Good
Excellent
Ideal

Cal/Val Network Design and Evolution

Copernicus Cal/Val Solution (EU H2020 CCVS) – With WGCV ACSG, IVOS and SAR participation

CCVS

Ground-based networks design

There is a need for R&D on *network design*, in particular for emerging measurement networks, but also for FRM-tailoring and sustainability of the existing networks.

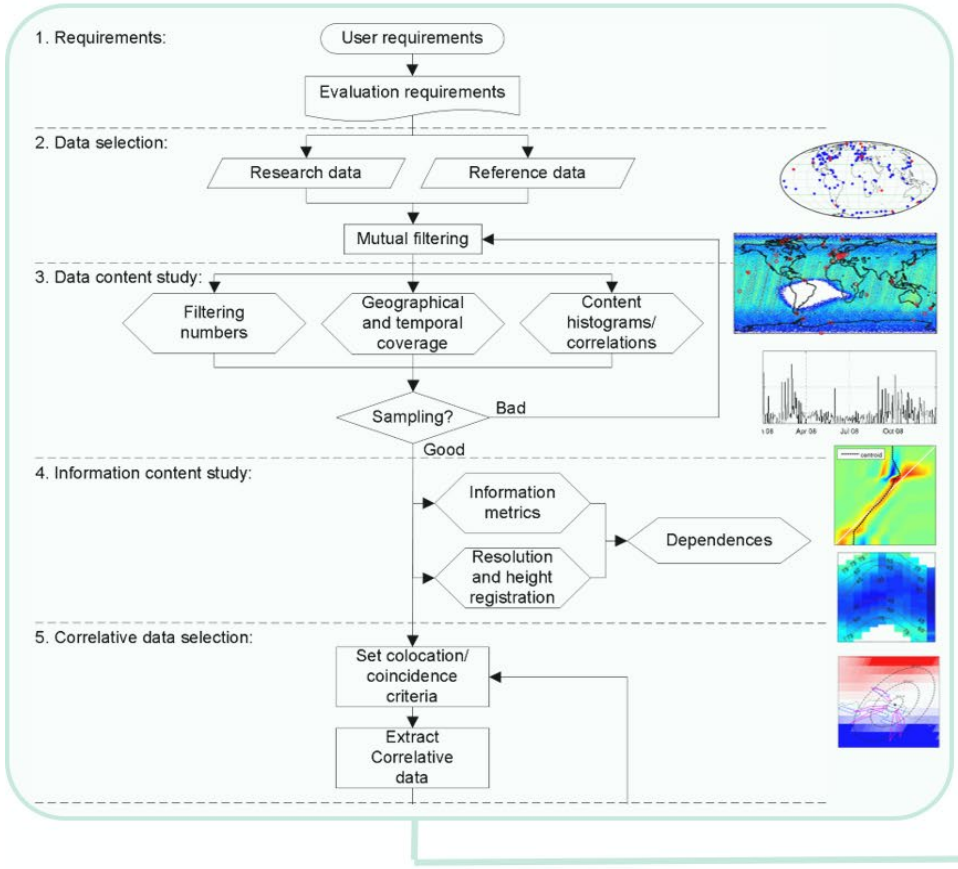
Cal/Val requirements => objective gap analysis criteria for Cal/Val infrastructures

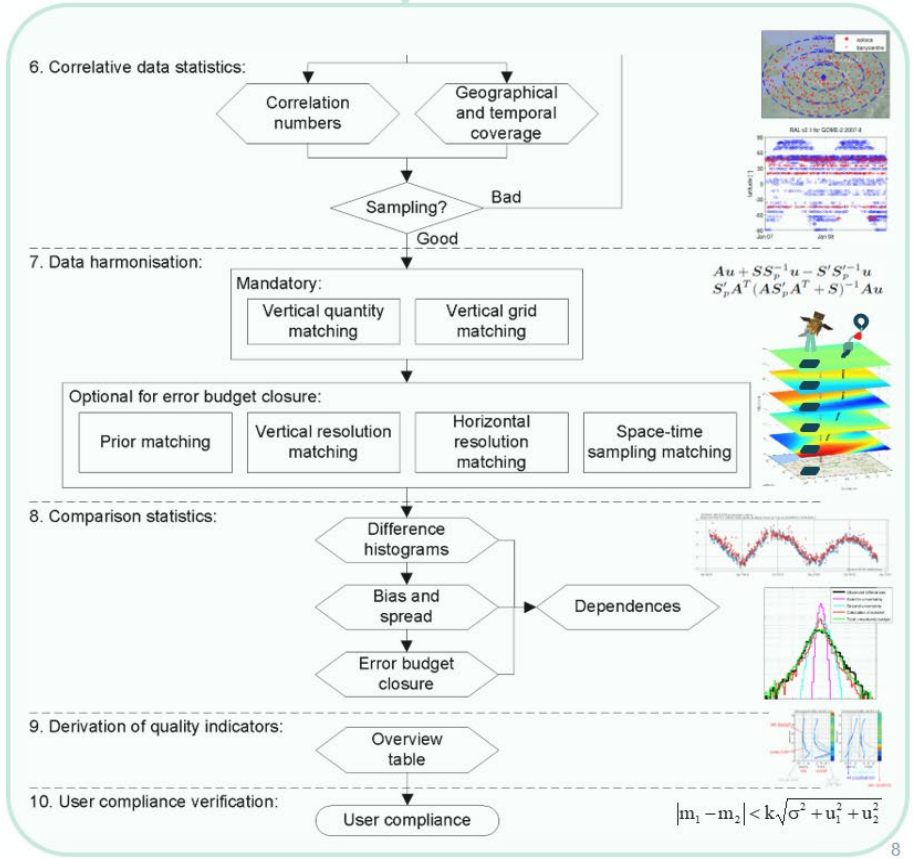
- Range of measurand
- Geographical coverage, types of atmospheric states (or regimes)
- Range and sampling of main influence quantities (SZA, T profile, surface albedo, aerosols, clouds…)
- Assessment of the spatio-temporal representativeness of measurements at a given location – requiring also assessment of spatio-temporal variability at that location => complementarity of airborne campaigns and modelling
- Co-location of instruments at 'supersites', e.g., SWIR with UVVIS, atmospheric composition and ancillary data (incl. surf. albedo) for in-depth validation of retrieval algorithms, validation of attribution proxies (simultaneous measurements of CO_2, NO_2, HCHO, SIF, smoke AOD)…

http://ccvs.eu

Maturity of Validation Method

Generic round-robin & validation protocol for atmospheric composition data





+ uncertainty propagation

Keppens *et al.*, AMT 2015

Presented at CEOS AC-(V)C 2014, College Park

Maturity of Validation Method

Operation	Input	Task	Output
1. Design of the validation study	Data quality requirements	Design validation objectives: quality indicators to produce, domains and ranges to address…	Set-up of following steps, including set of targeted quality indicators
2. Data selection and post-processing	Original datasets, quality flags, usage recommendations …	Quality screening of satellite and validation data sets	Original datasets + cleared datasets
3. Data content analysis	Original and cleared satellite datasets	Analysis of satellite data set	Validity of quality flags, identification of geographical/time coverage and horizontal resolution
4. Information content analysis	Averaging kernels, a priori profiles, covariance	Algebraic analysis of vertical averaging kernel matrixes: eigenvectors, DFS, Backus-Gilbert spread…	Information content metrics, vertical sensitivity and resolution, height registration
5. Spatio-temporal co-location	Cleared satellite and validation data sets, co-location criteria	Identification and extraction of co-located data pairs, optimisation of overlap between datasets	Co-located satellite and validation datasets and metadata
6. Co-location analysis	Co-located pairs dataset and metadata	Analysis of co-located pairs and associated parameters (influence quantities, ancillary data…)	Identification of geographical/time coverage of co-locations, of the covered ranges of measurand and influence quantities etc.
7. Data harmonisation	Co-located pairs dataset, associated averaging kernels, a priori and covariance	Change in coordinates, regridding, vertical and horizontal smoothing…	Co-located satellite and validation datasets with comparable vertical grid and reduced representativeness differences, ready for comparison
8. Data comparison and analysis	Cleared, co-located, harmonised datasets	Visual comparison of time series and maps, quantitative comparison of measurand values as a function of time, classified by range of influence quantity…	Time series, maps, histograms, oscillations, statistical estimates (bias, spread, drift…)
9. Quality information	Outcome of previous step	Sum up the findings of the previous steps, assign to every targeted quality indicator a range of values	List of qualitative and quantitative quality indicators, statements and recommendations
10. Acceptance	All results above, quality criteria (e.g. mission requirements)	Verification of satellite data quality compliance with mission and/or user requirements	Consistency of the co-located data sets, compliance with mission/user requirements, validity of ex-ante uncertainty estimates (systematic and random effects)
11. Reporting	All results above, quality criteria (e.g. mission requirements)	Reporting of validation; method, datasets, derived quality indicators	Reporting
12. Feedback	Validation report, intermediate results	Collect feedback from validation activities, audit validation process	Feedback to validation stakeholders: FRM data providers, infrastructure

Maturity assessment process for AC Validation Methods based on

- Round-robin generic protocol (Keppens et al., *AMT* 2015)
- Validation across EO domains (Loew et al., *Rev. Geophys.* 2017)

Maturity assessment of validation methods for Sentinel-4/5p/5 & CO2M data products

(Verhoelst et al., CCVS D3.2, 2022)

CCVS Product	Design	Data selection	Data content	Information content	Co-location	Co-location content	Harmonization	Comparison	QI	Acccptance	Reporting	Feedback
L1b												
Ozone (O_3) total column												
Ozone (O_3) tropospheric column												
Ozone (O_3) vertical profile												
Nitrogen dioxide (NO_2) (sub-) columns												
Formaldehyde (HCHO) column												
Glyoxal (CHOCHO) column												
Sulfur dioxide (SO_2) column												
Carbon monoxide (CO) column												
Methane (CH_4) column												
Carbon dioxide (CO_2) column												
Water vapor (H_2O) column												
Cloud properties												
Lambertian Equivalent Reflectivity (LER)												
Surface albedo												
Aerosol AOD												

Validation Protocol for Aerosols and Cloud Profiles

- CEOS CV-22-01: Validation protocols for atmospheric aerosol and cloud profiles
  See Th-05 presentation by R. Koopman
- Coordinator: R. Koopman (ESA/ESTEC). Agencies: ESA, NASA, JAXA and EUMETSAT, group expanding with 83 contributors at present
- ESA-JAXA EarthCARE workshop, ESA/ESRIN, 13-17 Nov. 2023

Limb Sounding Constellation

Recent launches

- MATS (L 2022/11)
- NOAA-21 OMPS-LP (L 2022/11)

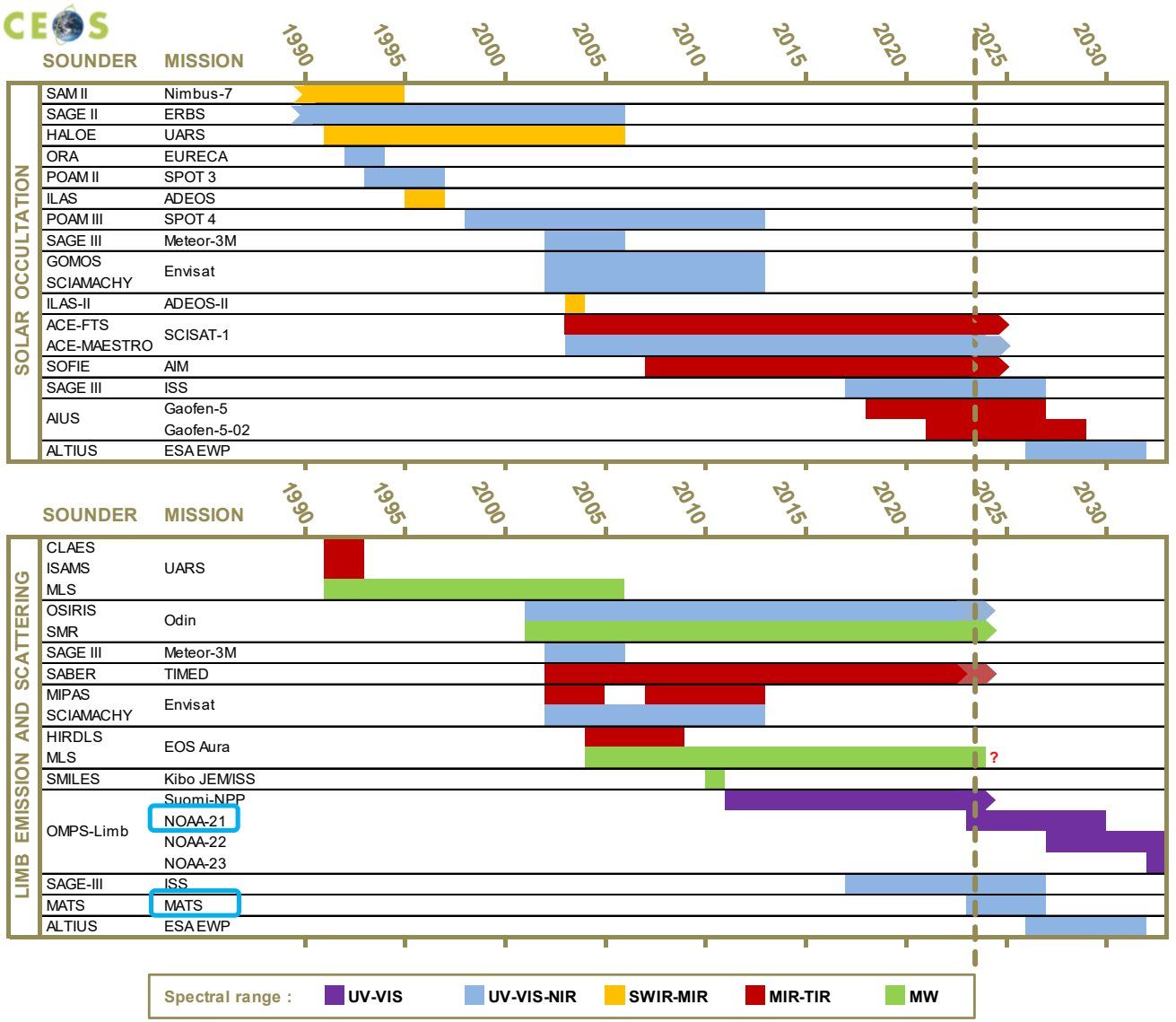
Upcoming missions

- ARGOS (L 2024/Q2)
- ALTIUS (L 2026/03)

Developments

- C-MLS, SMILES-2
- CAIRT (candidate EE-11)
- SAGE IV, CubeMAP
- HAWC ALI, TICFIRE and SHOW

Validation challenges: mesosphere, H_2O, aerosols and clouds, dynamics/waves, 3D/tomography, operational validation for DA & services, constellations

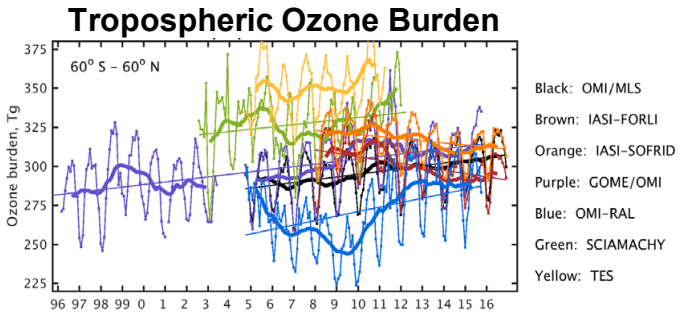


Tropospheric Ozone Constellation

IGAC Tropospheric Ozone Assessment Report-II

Questions from TOAR-I (Gaudel *et al.*, 2018)

- Why do measured distributions and trends differ (i) among satellites, and (ii) w.r.t. monitoring networks ?
- Differences in vertical sensitivity and sampling ?
- Differences in tropopause column definition ?
- (In)consistencies with TOST (ozonesonde based trajectories) ?



TOAR tropospheric ozone assessment report

➢ **CEOS response:** VC-20-01 - Tropospheric ozone dataset validation and harmonization

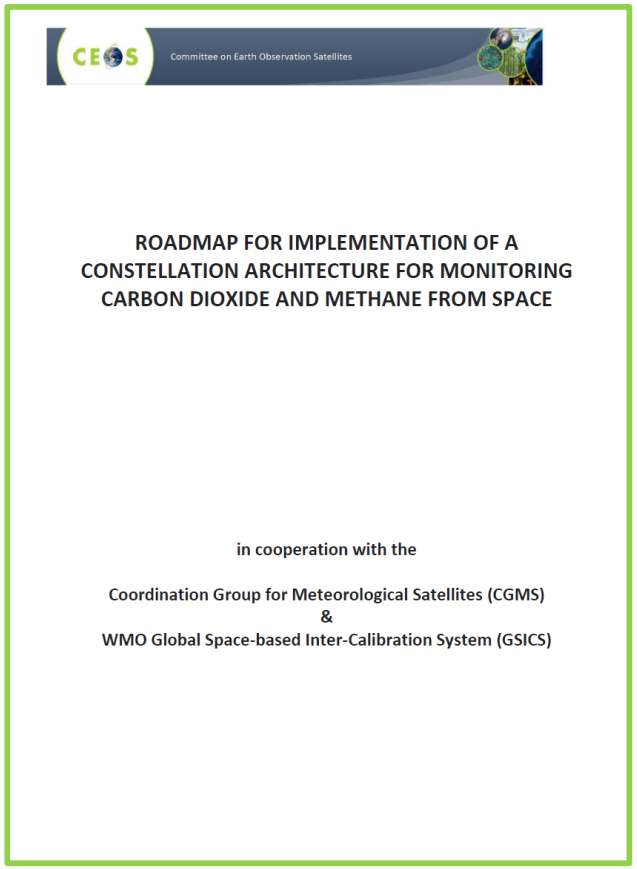
- Coordinator: D. Loyola (DLR); support G. Labow (NASA) & J.-C. Lambert (BIRA-IASB)
- 15+ participating agencies
- Participation in TOAR-II Satellite Ozone WG
- Participation in SPARC TUNER (Towards Unified Error Reporting)
- Status: reports in the Tropospheric Ozone session this afternoon *(talks Th-12 to Th-18)*

SPARC TUNER TOWARDS UNIFIED ERROR REPORTING

GHG Satellite Constellation

GHG constellation roadmap – Annex C: Implementations actions – Calibration & Validation

AREA	ACTION ID	ACTION DESCRIPTION
Calibration & Validation	CV-1	Address existing CEOS Action by Q1 2020 on "Greenhouse gas reference standards for interoperability": Develop a list of **reference standards for CO_2 and CH_4 products** that are suitable for use in inter-comparison of multiple missions.
	CV-2	Identify the current **shortcomings/gaps/sustainability in GHG calibration and validation capabilities**, and formulate recommendations on the medium- to long-term way forward, that is with a specific focus on GHG Fiducial Reference Measurement (FRM).
	CV-3	Identify gaps and suggest improvements in the **inter-calibration of a future LEO/GEO constellation of GHG sensors**
	CV-4	Define **protocols for comparing and validating GHG retrieval algorithms**
	CV-5	Identify gaps and suggest improvements in **ground-based and airborne validation infrastructure** (i.e. geographical/geophysical gaps for FRM) and other long-term validation needs (at horizon 2025-on).
	CV-6	Work towards an **operational reporting on the quality of space-borne GHG measurements** and the underlying calibration and validation infrastructure.
	CV-7	Identify a repository for hosting quality-controlled CO2 and CH4 products - see Rec#13: CEOS and CGMS agencies should consider a [centralized or possibly geographically distributed] repository for hosting quality-controlled CO2 and CH4 products, with internal capability for product inter-comparison



v2.3, March 2020
Update in progress

GHG Satellite Constellation

GHG constellation roadmap v2.3 – Annex C: Implementations actions – Calibration & Validation

CV-2 Identify the current shortcomings/gaps/sustainability in GHG calibration and validation **capabilities**, and formulate recommendations on the medium- to long-term way forward, that is with a specific focus on GHG Fiducial Reference Measurement (FRM).

CV-5 Identify gaps and suggest improvements in ground-based and airborne validation **infrastructure** (i.e. geographical / geophysical gaps for FRM) and other long-term validation needs (at horizon 2025-on)

https://events.spacepole.be/event/160/

See Talk Tu-18 by M.K. Sha

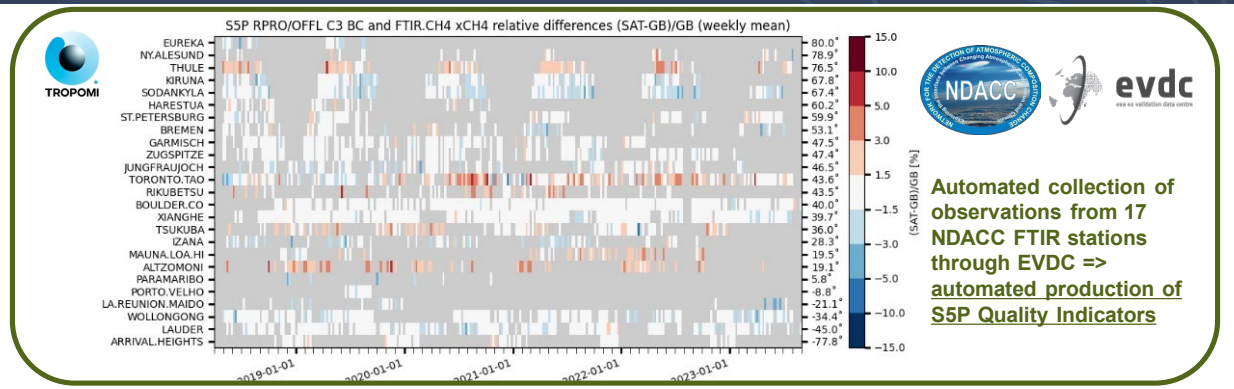
GHG Satellite Constellation

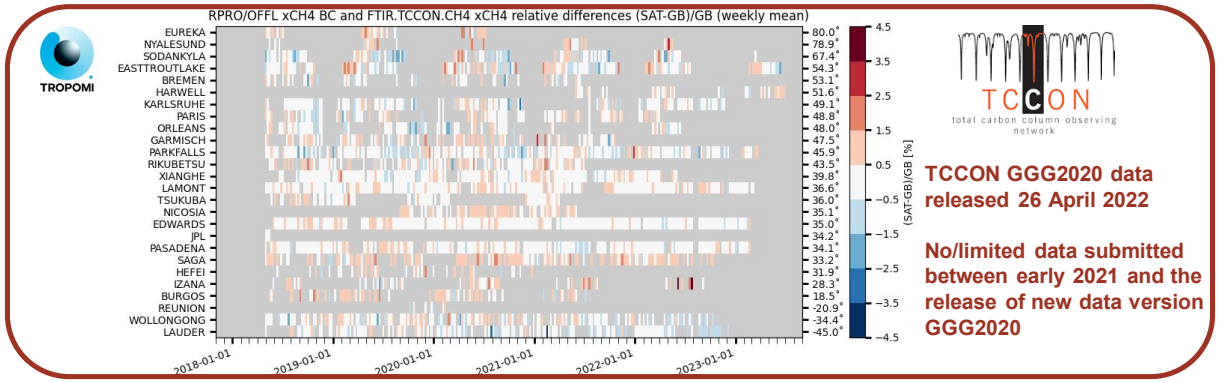
GHG constellation roadmap – Annex C: Calibration & Validation

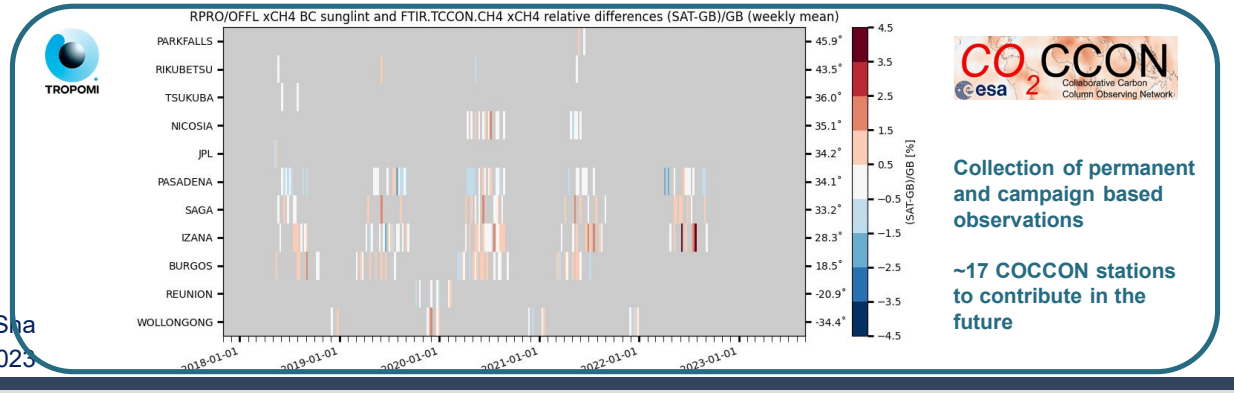
CV-6 Pathfinder: ESA/Copernicus ATM-MPC Sentinel-5P TROPOMI CH_4 and CO operational validation based on three GHG column/profile monitoring networks

- **NDACC FTIR** : automated validation channel in ATM-MPC Automated Validation Server (https://mpc-vdaf-server.tropomi.eu).
  Validation protocols based on published experience with HALOE, MOPITT, SCIAMACHY, MIPAS, ACE-FTS, IASI, GOSAT…
- **TCCON FTIR** : manual validation channel in ATM-MPC, ESA contract for operations support to be placed
- **COCCON FTIR** : manual validation channel in ATM-MPC, EVDC data collection and automation in progress (ESA contract 2023-2027)

S5P TROPOMI CH_4 & CO validation updated permanently vs. **NDACC FTIRs** and monthly – when and where data available – vs. **TCCON** & **COCCON** FTIRs.
Quarterly validation reports available on http://mpc-vdaf.tropomi.eu







CH_4 images courtesy M.K. Sha
ATM-MPC review October 2023

GHG Satellite Constellation

GHG constellation roadmap v2.3 – Annex C: Implementation Actions – Calibration & Validation
Recommendations to CEOS SIT TW 2023 for Cal/Val networks capabilities, infrastructure and operational capacity

1. **NETWORKS DESIGN AND EVOLUTION:** to support gap analysis studies with a view to tailoring CO_2,CH_4 and N_2O networks deployments to Cal/Val needs of the GHG satellite constellation: background/hot spots, land/ocean, low/high albedo, full range of atmospheric temperature…
2. **INSTRUMENT DEPLOYMENT:** (i) to further develop (low-cost, light-weight, mobile) low-resolution infrared instruments; (ii) to support standardized production of enclosures for their deployment in the field; (iii) to maintain a supply of spare parts.
3. **CALIBRATION:** to support the development of and maintain mutually consistent calibration and QA/QC of the GHG Cal/Val networks – within and across networks. Key actions: (i) traceability towards internationally agreed standards; (ii) more regular and network-wide deployment of traveling standard; (iii) more regular intercomparisons within and across networks, and between in situ (AirCore…) and remote sensing (networks); (iv) facilitate AirCore deployment; (v) establish a central AirCore data archive.
4. **DATA PROCESSING:** to support GHG Cal/Val network data processing improvements needed to maintain FTIR data precision/accuracy and meet future goals: formal intercomparison exercise of the GGG and PROFFAST retrieval algorithms, development and standardization of profile retrievals, spectroscopy studies.

GHG Satellite Constellation

GHG constellation roadmap v2.3 – Annex C: Implementation Actions – Calibration & Validation
Recommendations to CEOS SIT TW 2023 for Cal/Val networks capabilities, infrastructure and operational capacity

5. **DATA ACCESS:** to establish interoperable GHG Constellation Cal/Val Data archives and tools for tailored network data (traceable, open, metadata, co-located…) and 'hidden' data (e.g. campaigns), ideally coupled to New Space related matchup database(s).
6. **TIMELINESS:** to organize concertation between stakeholders and with networks data providers to support rapid and continuous availability and improved access to networks-wide GHG data.
7. **CENTRAL PROCESSING FACILITIES (CPF):** to establish central processing facilities for every network product, which will directly support harmonized calibration **(3)**, data processing, QA/QC and tailoring **(4-5)** and timeliness **(6)**.
8. **GHG EMISSIONS AND ATTRIBUTION:** to support the development of new Cal/Val protocols for satellite derived GHG emissions and fluxes, in collaboration with relevant bodies and initiatives (global stocktakes, WMO GGGW, UNEP IMEO, New Space…) Consider co-located measurements of GHG and tracers of anthropogenic/biogenic contributions for better attribution of emissions.

Air Quality Constellation

VC-20-02	Air quality constellation validation coordination	2024 Q4	AC-VC WGCV
VC-20-03	Air quality constellation validation coordination: validation plans	2022 Q4	AC-VC WGCV
VC-20-04	Air quality constellation validation coordination: announcements of opportunity	2023 Q4	AC-VC WGCV

Cal/Val coordination (VC-20-02), plans (-03), Announcements of Opportunities (-04)

See presentations in Wednesday morning AQ Session

- GEMS AO (issued 2018) → Cal/Val activities with international participation, ESA PEGASOS routine validation service, comparisons with Sentinel-5P, testing of Sentinel-4 L2 algorithms
- TEMPO (L 2023/04), Mission Validation Plan, joint NASA/NOAA summer 2023 field campaigns
- Sentinel-4/5 Cal/Val AO Call to be issued end 2023

- New Pandora products (SO_2, HCHO, O_3), growing Pandora Asian Network complementing Pandora Global Network for operational acquisition of reference data
- CINDI-3 field campaign (2024/05-06): MAX-DOAS inter-calibration, aerosols, tomography…
- NDACC FTIR network expanding to/operationalizing for new species: HCHO, NH_3…

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.

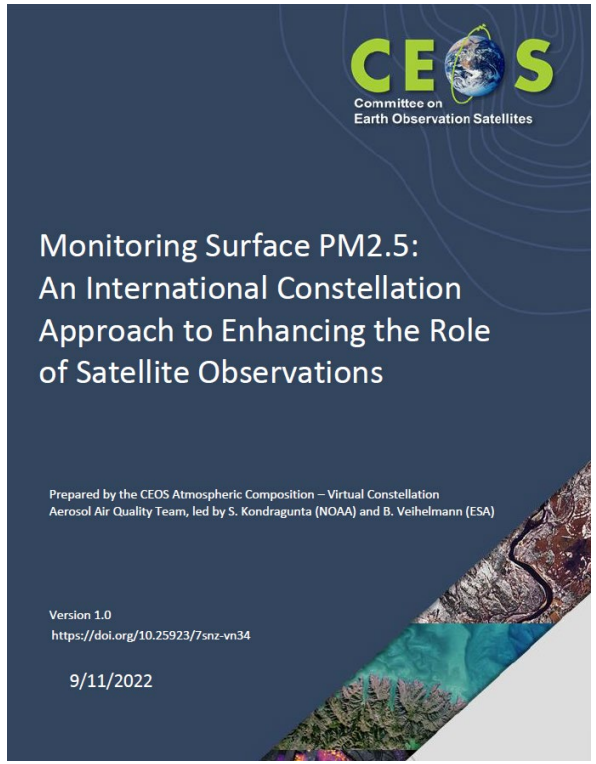
Next steps:
roadmap, gap analysis

Air Quality Constellation – Surface PM2.5

- Whitepaper “Monitoring Surface PM2.5” (VC-20-05) endorsed at plenary 2022
- Cal/Val related recommendations:

6. Continue efforts to establish, monitor, and enhance the radiometric calibration consistency of space-borne multispectral imagers. Continue and strengthen related efforts made by the Global Space-based Inter-Calibration System (GSICS).

14. Collect and analyze comprehensive reference data sets including measurements from ground-based in-situ PM sensors and co-located radiometers and ceilometers, in order to enhance the understanding of the link between satellite observables and near-surface PM concentrations.
15. Validate satellite-informed PM products, using ground-based in-situ PM data from operational networks. Pursue extending the source of PM reference data by calibrating low-cost $PM_{2.5}$ sensors and developing correction methodologies.
16. Create a data center for providing access to validation data.



Next steps: Cal/Val needs → roadmap

Cal/Val for the Constellations

12:00 - 13:00	Th-11 - Panel review of Cal/Val needs for the AER, GEO-AQ and GHG constellations. Discussion on the way forward (suggestions): need for framework documents, Cal/Val protocols, Task Teams, match-up databases, field activities…? General Q&A, wrap-up