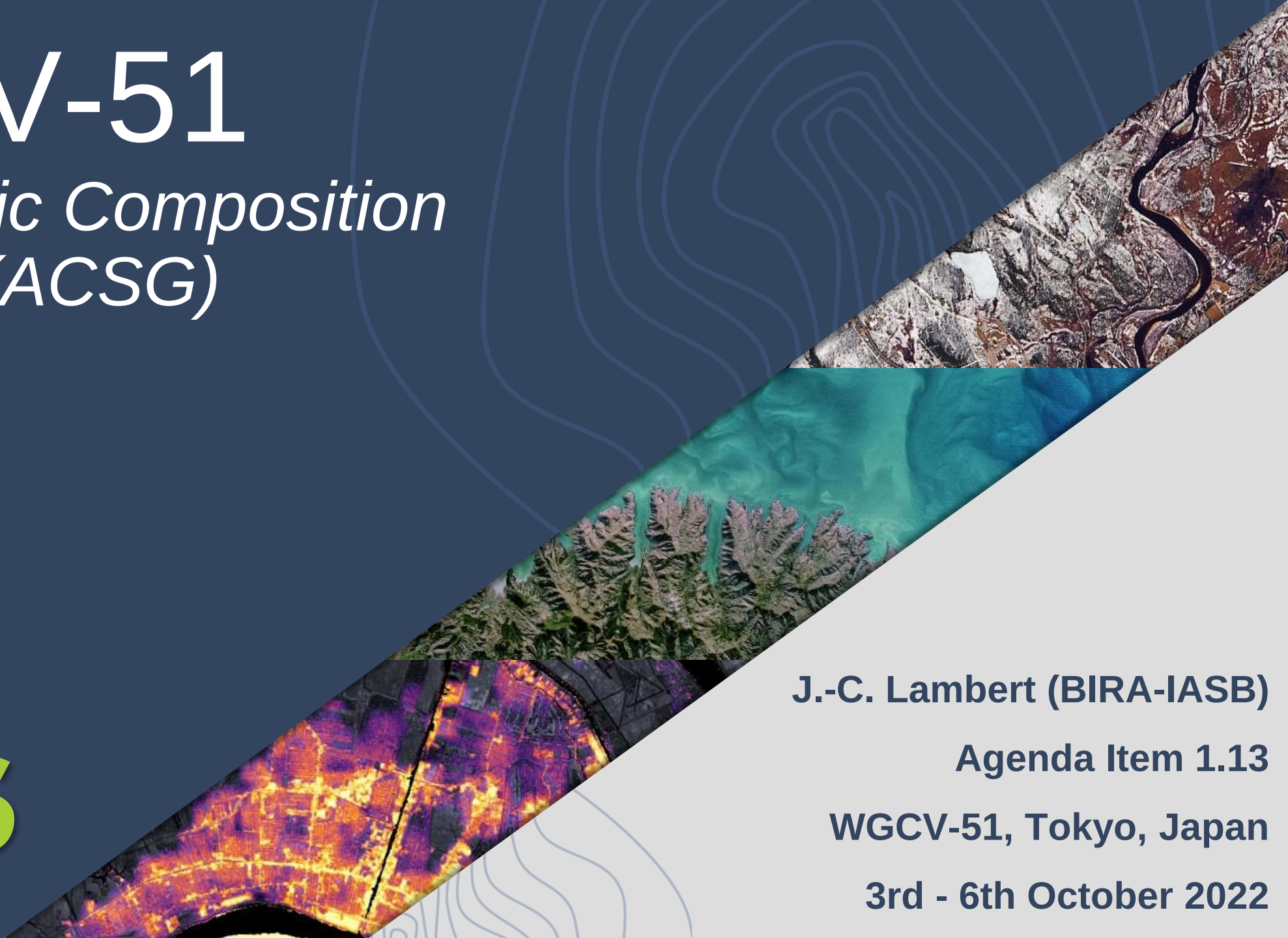
WGCV-51

Atmospheric Composition Subgroup (ACSG)



CEOS
Committee on
Earth Observation Satellites

J.-C. Lambert (BIRA-IASB)

Agenda Item 1.13

WGCV-51, Tokyo, Japan

3rd - 6th October 2022

ACSG Update

- New ACSG Chair: J.-C. Lambert’s candidature
- New ACSG Vice-Chair: consultations ongoing
- Review of membership (by agency) in progress
- Next ACSG meeting proposed for 2023
- Questionnaire circulated for topics of discussion

ACSG Topics

- Potential topics of interest
  - New validation best practices for atmospheric aerosol and cloud profiles (CV-22-01).
  - Enhanced dialogue with FRM/validation data providers.
  - Strengthen cooperation with AC-VC for coordinating the validation for the GEO-AQ and GHG Constellations.
  - PICS-based evaluation of L1B (IR & RA) data measured by nadir atmospheric sounders in the UV, VIS, NIR and SWIR.
  - Exchanges of best practices on operational validation systems.
  - Others?

Enhanced dialogue with FRM data providers (1)

- Enhanced dialogue with ground-based monitoring networks necessary to identify existing issues and gaps in reference measurements, validation methods and validation resources, and discuss potential solutions
  - On the agenda of *CCVS In-situ workshop* and *NDACC Steering Committee 2022*

- Copernicus Cal/Val Solution "In-situ" Workshop (May 9-11, 2022, online event)
  - Participation: several networks and campaign delegates, Copernicus Office, EEA, ESA, EUMETSAT, other agencies, Sentinel MPCs, operational services, GSICS
  - General sessions incl. discussion panels
  - Parallel thematic sessions, among these Atmospheric Composition
  - Further discussions in CCVS Agora at ESA Living Planet Symposium 2022 (Bonn, 2022/05)

Enhanced dialogue with FRM data providers (2)

NDACC Steering Committee meeting 2022 (Sept. 26-30, Paris, hybrid)

- Participants
  - NDACC WGs Chairs: Brewer/Dobson, DIAL, FTIR, MW, sondes, spectral UV, UVVIS
  - Space agencies delegates: ESA, EUMETSAT, NASA, NIES, NOAA
  - Cooperating networks representatives: AERONET, AGAGE, BSRN, EUBREWNET, GAW, GRUAN, HATS, MPLNET & GALION, PGN, SHADOZ, TCCON
- ACSG relevant agenda topics:
  - Satellite WG Report 2022 – incl. presentation of CEOS WGCV/ACSG and AC-VC updates
  - Presentation of CCVS outcome in atmospheric domain
  - Discussion on FRM maturity of NDACC measurements
- Actions taken:
  - Satellite WG (incl. ACSG members) to better define FRM criteria in AC domain
  - Instrument WGs to develop and apply tentatively a FRM maturity evaluation system (matrix?) applicable to all NDACC instruments

Enhanced dialogue with FRM data providers (3)

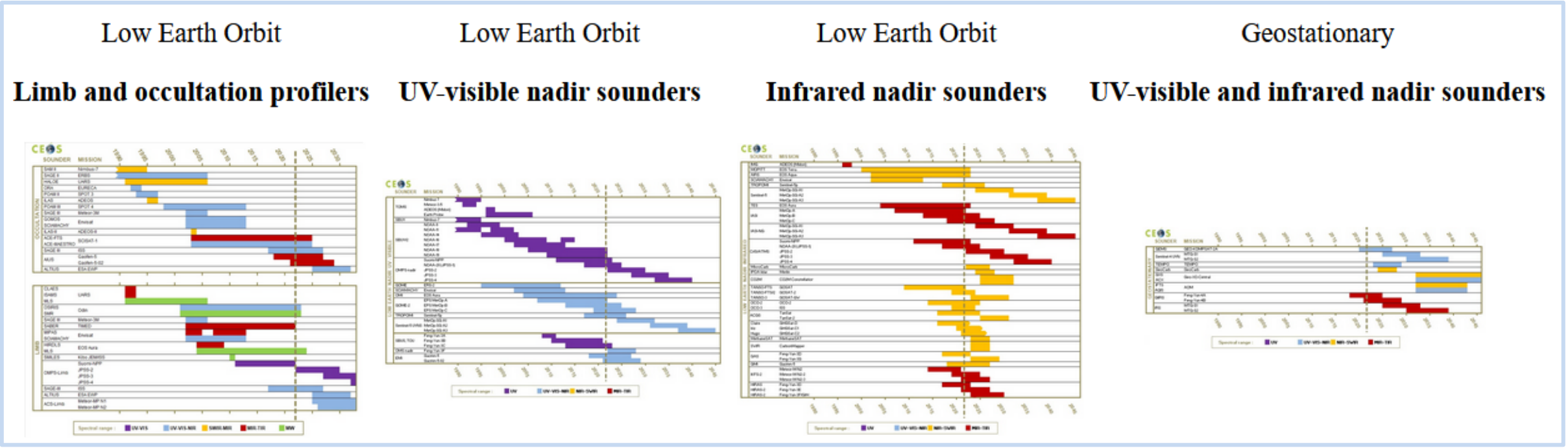
- Challenge of securing stable funding for ground-based measurements.
- Travelling SI standards to ensure a common traceability across a measurement network or between different networks.
- Timely involvement of metrology and spectroscopy communities.
- Central instrument calibration, characterization and maintenance facilities whenever industrial instrument providers do not perform those operations.
- Need for a validation maturity matrix aiming at the evaluation of fitness-for-purpose of the Cal/Val process (not the validation results for a specific dataset, but the validation methods and data for a generic data product).
- Characterization of measurement sites, e.g., with airborne campaigns to characterize homogeneity over site and horizontal/vertical representativeness.
- Need for overall collaboration among Networks, aerial campaigns, RIs, agencies, services, CEOS, WMO SC MINT/ET-QTC…

NDACC Satellite WG website update

access via main website https://ndacc.org

and https://accsatellites.aeronomie.be

- Directory of relevant atmospheric composition (trace gases) satellite missions
- Downloadable mission time charts

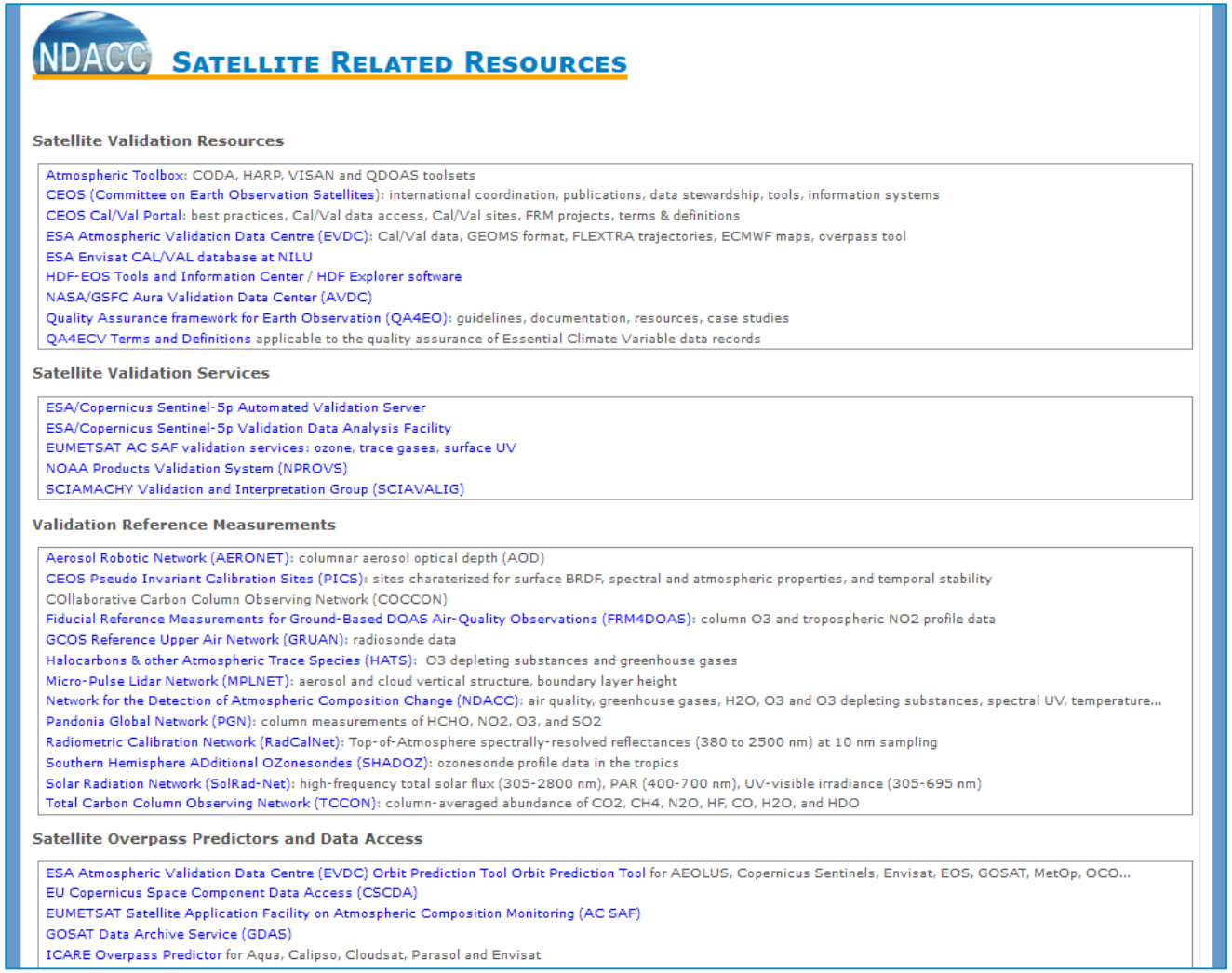


AI Synergies Cal/Val Portal and NDACC Satellite Website (2)

NDACC Satellite WG website new features

- Resources page:
  - Validation resources
  - Validation services
  - Validation reference measurements
  - Overpass predictors and data access

Exchanges with Cal/Val Portal in progress. WGCV-50-ACT-05



NDACC SATELLITE RELATED RESOURCES

Satellite Validation Resources

Atmospheric Toolbox: CODA, HARP, VISAN and QDOAS toolsets
CEOS (Committee on Earth Observation Satellites): international coordination, publications, data stewardship, tools, information systems
CEOS Cal/Val Portal: best practices, Cal/Val data access, Cal/Val sites, FRM projects, terms & definitions
ESA Atmospheric Validation Data Centre (EVDC): Cal/Val data, GEOMS format, FLEXTRA trajectories, ECMWF maps, overpass tool
ESA Envisat CAL/VAL database at NILU
HDF-EOS Tools and Information Center / HDF Explorer software
NASA/GSFC Aura Validation Data Center (AVDC)
Quality Assurance framework for Earth Observation (QA4EO): guidelines, documentation, resources, case studies
QA4ECV Terms and Definitions applicable to the quality assurance of Essential Climate Variable data records

Satellite Validation Services

ESA/Copernicus Sentinel-5p Automated Validation Server
ESA/Copernicus Sentinel-5p Validation Data Analysis Facility
EUMETSAT AC SAF validation services: ozone, trace gases, surface UV
NOAA Products Validation System (NPROVS)
SCIAMACHY Validation and Interpretation Group (SCIAVALIG)

Validation Reference Measurements

Aerosol Robotic Network (AERONET): columnar aerosol optical depth (AOD)
CEOS Pseudo Invariant Calibration Sites (PICS): sites charaterized for surface BRDF, spectral and atmospheric properties, and temporal stability
COllaborative Carbon Column Observing Network (COCCON)
Fiducial Reference Measurements for Ground-Based DOAS Air-Quality Observations (FRM4DOAS): column O3 and tropospheric NO2 profile data
GCOS Reference Upper Air Network (GRUAN): radiosonde data
Halocarbons & other Atmospheric Trace Species (HATS): O3 depleting substances and greenhouse gases
Micro-Pulse Lidar Network (MPLNET): aerosol and cloud vertical structure, boundary layer height
Network for the Detection of Atmospheric Composition Change (NDACC): air quality, greenhouse gases, H2O, O3 and O3 depleting substances, spectral UV, temperature...
Pandonia Global Network (PGN): column measurements of HCHO, NO2, O3, and SO2
Radiometric Calibration Network (RadCalNet): Top-of-Atmosphere spectrally-resolved reflectances (380 to 2500 nm) at 10 nm sampling
Southern Hemisphere ADditional OZonesondes (SHADOZ): ozonesonde profile data in the tropics
Solar Radiation Network (SolRad-Net): high-frequency total solar flux (305-2800 nm), PAR (400-700 nm), UV-visible irradiance (305-695 nm)
Total Carbon Column Observing Network (TCCON): column-averaged abundance of CO2, CH4, N2O, HF, CO, H2O, and HDO

Satellite Overpass Predictors and Data Access

ESA Atmospheric Validation Data Centre (EVDC) Orbit Prediction Tool Orbit Prediction Tool for AEOLUS, Copernicus Sentinels, Envisat, EOS, GOSAT, MetOp, OCO...
EU Copernicus Space Component Data Access (CSCDA)
EUMETSAT Satellite Application Facility on Atmospheric Composition Monitoring (AC SAF)
GOSAT Data Archive Service (GDAS)
ICARE Overpass Predictor for Aqua, Calipso, Cloudsat, Parasol and Envisat

GHG Roadmap → GHG Networks for Satellite Validation (1)

NDACC IRWG

http://ndacc.org

- Bruker 120HR/125HR
- Resolution 0.0036 cm-1
- Spectral range: SWIR, MIR and TIR
- Measurements every ±10’
- 21 stations worldwide
- Targets: O3, CH4, N2O, (CO2, HCHO, SF6, CFC, HCFC, H2O, HDO not official), CO, HNO3, HCl, HF, HCN, C2H6, ClONO2, (C2H2, PAN, OCS, CH3OH, NH3, HCOOH, NO2 not official)
- Profile retrievals (limited vertical resolution, typically tropo/strato partial columns)
- Retrieval software: SFIT or PROFFIT
- Some central processing in development in ACTRIS, QA/QC for selected targets in CAMS operational validation

TCCON

http://tccon.org

- Bruker 125HR
- Resolution 0.02 cm^{-1}
- Spectral range: SWIR
- Measurements every ~ 3’
- 28 stations worldwide
- Targets: CO_2, CH_4, N_2O, H_2O, HDO, CO, HF
- Profile scaling retrievals (profile retrievals in development)
- Retrieval software GGG
- Central QA/QC

COCCON

http://www.imk-asf.kit.edu/english/COCCON.php

- Bruker EM27/SUN
- Resolution 0.5 cm^{-1}
- Spectral range: SWIR
- Measurements every ~ 1’
- > 60 instruments worldwide (some fixed sites but mostly for campaigns)
- Targets: CO_2, CH_4, CO
- Profile scaling retrievals
- Retrieval software PROFFAST
- Central calibration & processing facility at KIT

Courtesy M. De Mazière, B. Langerock and M.K. Sha (BIRA-IASB)

GHG Roadmap → GHG Networks for Satellite Validation (2)

NDACC IRWG

- Operational use in: ESA MPC TROPOMI validation, CAMS validation (RD delivery supported by CAMS)
- Recent and ongoing harmonisation efforts in QA4ECV, GAIA-CLIM, CAMS27, C3S-311a-Lot3 (BARON)
  Upcoming SFIT/PROFFIT to improve harmonization of uncertainties evaluation, better spectroscopy
- Selected NDACC stations to join EU research infrastructure ACTRIS: with central processing facility, QA/QC, training…
- CO2 retrieval strategy under development (IUP/UB & BIRA-IASB)

TCCON

- Operational use in: OCO-2/3 & GOSAT/2 Cal/Val, CAMS validation, ESA TROPOMI validation (limited RD delivery)…
- GGG2020 show improved prior profiles (shape and possible bias), no CO calibration factor, improve spectroscopy, reduce remaining airmass and H_2O dependences, reduce scatter in CO product, improve diagnostics for instrumental issues.
- Negotiations ongoing for selected TCCON stations to join EU research infrastructure ICOS, with central processing facility
- Profile retrievals under development. Tropospheric partial columns can be derived indirectly

COCCON

- Operational usage in: OCO-2/3, GOSAT/2, S5P TROPOMI validation (started in 2020)…
- Planned update foreseen for PROFFAST, redefined spectroscopic descriptions + improved line lists
- EM27/SUN as travelling standard for TCCON, COCCON can complement TCCON, support by ESA for COCCON-PROCEEDS, follow-up crucial for current capabilities of COCCON
- Towards extension of COCCON with VERTEX70 and IRcube (2 other low resolution FTIR instruments – with higher spectral resolution and additional species) – ESA FRM4GHG project
  https://frm4ghg.aeronomie.be

Courtesy M. De Mazière, B. Langerock and M.K. Sha (BIRA-IASB)

GHG Roadmap → GHG Networks for Satellite Validation (3)

New developments:

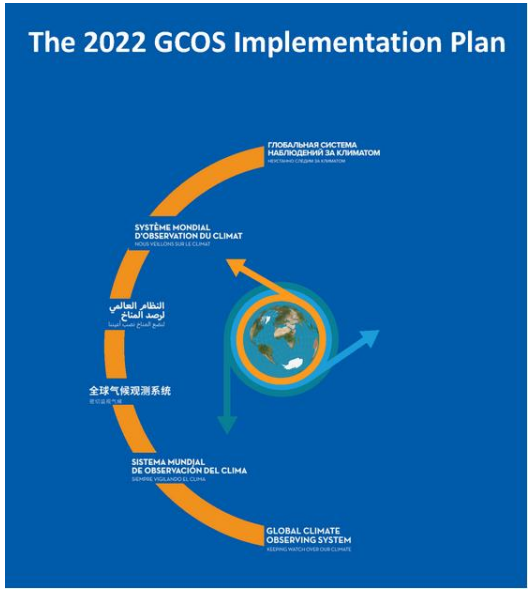
- Retrieval of CH4 vertical profile information from TCCON NIR spectra with 2.4 DOFs (https://doi.org/10.5194/amt-12-6125-2019) – EU H2020 – RINGO
- Retrieval of CH4 and N2O total columns from low-resolution (0.2 cm-1) Bruker Vertex70 in the mid-infrared region (https://doi.org/10.5194/amt-2022-17); first comparison of HCHO retrievals with high-resolution show promising results, further improvements under testing.
- Traveling standard instrument operating autonomously for NIR using EM27/SUN developed and already deployed at TCCON stations in Japan, Canada, next will be Australia.
- Development of autonomous mobile set-up for field deployment of low-resolution spectrometers – compact solar tracker, Stirling-cooled InSb detector for MIR measurements.
- Fiber optics feed for coupling solar radiation to low-resolution spectrometers (IRCube, EM27/SUN, …).
- Develop AirCore observation of additional species (N2O, OCS). – ESA FRM4GHG project https://frm4ghg.aeronomie.be

Important message !

Reference networks providing data for satellite validation lack structural funding. While some projects fund data del ivery, mosts station run on short term funding sources for operation, maintenance and data acquisition. This poses question on the long-term operation of the site and the availability of reference data.

Review of GCOS Implementation Plan 2022

CMRS-22-04 Comment and support the draft GCOS Implementation Plan 2022



- Participation of several ACSG members in the draft GCOS IP 2022 public review (May 2022) and in WMO Rolling Review of Requirements activities.

- SIT 2022 D4 and B1 – Cf. enhanced dialogue with COCCON, NDACC, TCCON…
  - Need for a central database of ground-based validation data, preferably mirroring network data archives
  - Central database should collect network calibration details and resources (e.g., database of airborne and AirCore soundings…)

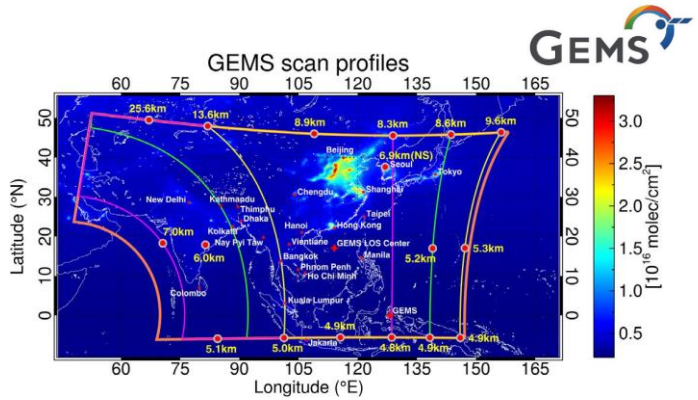
Cal/Val in AC-VC #18 Meeting

- AC-VC-18 (March 14-18, 2022) planned in Brussels, turned into an online event https://events.spacepole.be/event/126
- Agenda
  - Air Quality: Aerosols (Lead S. Kondragunta, NOAA)
  - Air quality: Trace gases (Leads B. Lefer, NASA, B. Veheilmann, ESA)
  - Greenhouse gases, emission inventories for global stocktakes (Lead J. Worden, JPL)
  - Ozone (Lead D. Loyola, DLR)
  - Science serving society, interdisciplinary, multi-species
- Cal/Val presentations embedded in thematic sessions; seed questions on Cal/Val in discussion time slots.

Air Quality Constellation Validation Coordination (1)

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

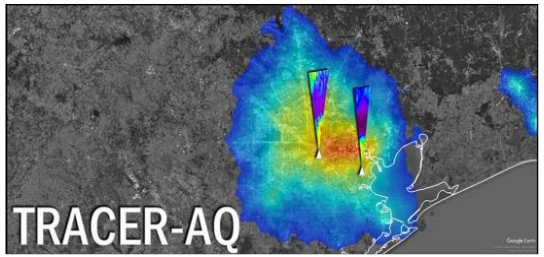
- Coordinator B. Veihelmann (ESA)
- Agencies: ESA, EUMETSAT, IASB-BIRA, NASA, NIER, SAO…
- AC-VC / WGCV joint document GEO-AQ Satellite Constellation Geophysical Validation Needs
- Coordinated ESA/NASA support to PGN developments
- Joint participation in ground/airborne field campaigns, e.g., CINDI-3 at Cabauw (NL) in September 2023
- AO calls: operational/being drafted
  - EU and US responses to NIER AO for GEMS Validation Team
  - ESA PEGASOS: Sentinel-5p MPC validation service application to GEMS validation

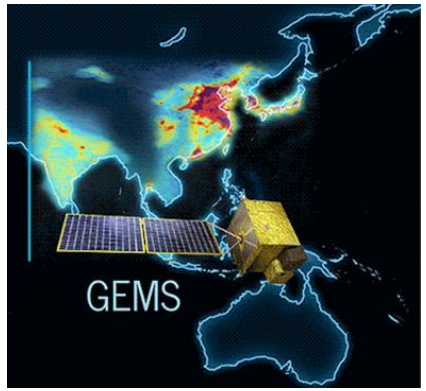


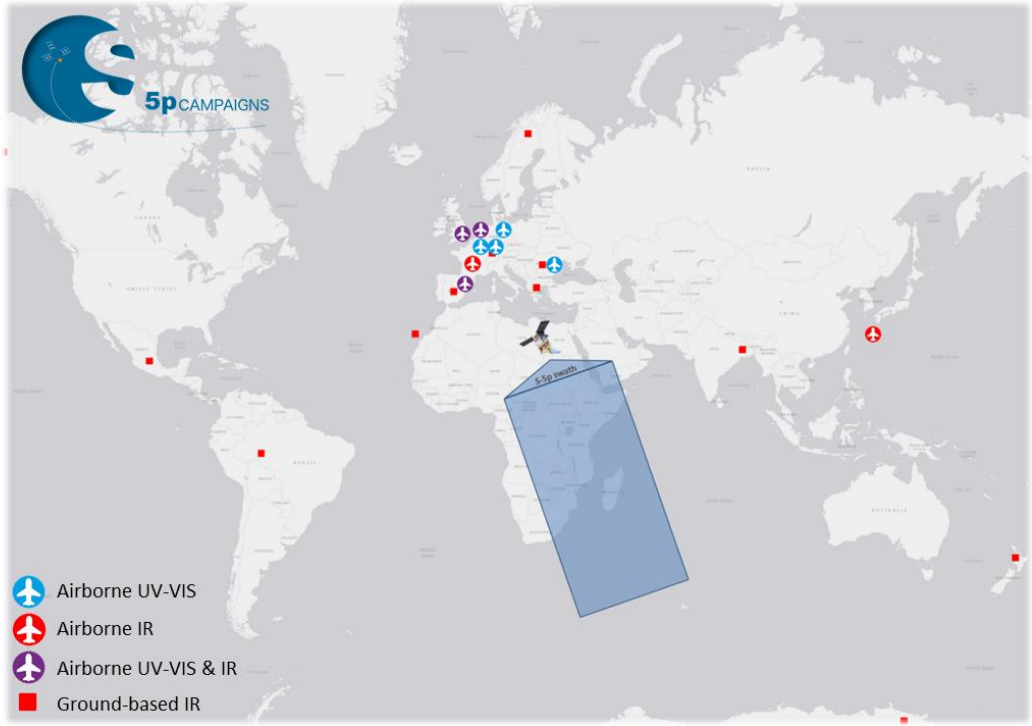
Air Quality Constellation Validation Coordination (2)

AC-VC-18, Air Quality Trace Gases Session (2022/03)

	Calibration/Validation of AQ Observations	
3.09	S5P/TROPOMI AQ Products Cal/Val Status	Jean-Christopher Lambert (BIRA)
3.10	Pandora Asia Network for Air Quality Diagnosis and GEMS Validation	Limseok Chang (NIER)
3.11	GMAP2021 Campaign, MAX-DOAS and Pandora Consistency, GOSAT-GW Validation Plan	Yugo Kanaya (JAMSTEC)
3.12	ASIA-AQ Campaign Plans	Jim Crawford (NASA)
3.13	AEROMMA Campaign: Objectives for TEMPO Validation	Brian McDonald (NOAA)
3.14	EPA Efforts on Preparing for TEMPO Validation	Luke Valin (US EPA), Jim Szykman (US EPA)
	Discussion	
3.15	what to do to make the satellite products more useful? issues related to assimilating AQ trace gas products into AQ forecasts multi-sensors synergy for AQ trace gas observation? exploring the relationship between AQ trace gases and GHGs and value to the Global Stocktake WGCV-atmospheric sub-group	All





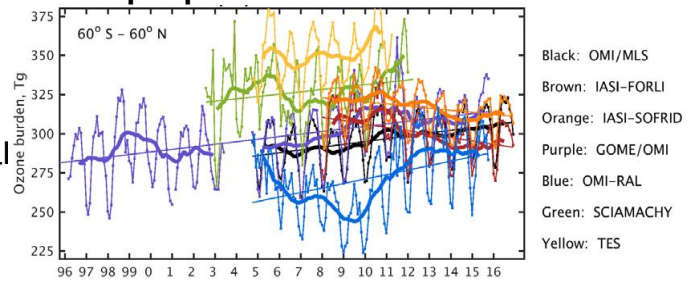


IGAC Tropospheric Ozone Assessment Report

- **Questions from TOAR-I** **(Gaudel *et al.*, 2018)**
- Why do measured distributions and trends differ (i) among satellites, a
- Differences in vertical sensitivity and sampling ?
- Differences in tropopause column definition ?
- (In)consistencies with TOST (ozonesonde based trajectories) ?

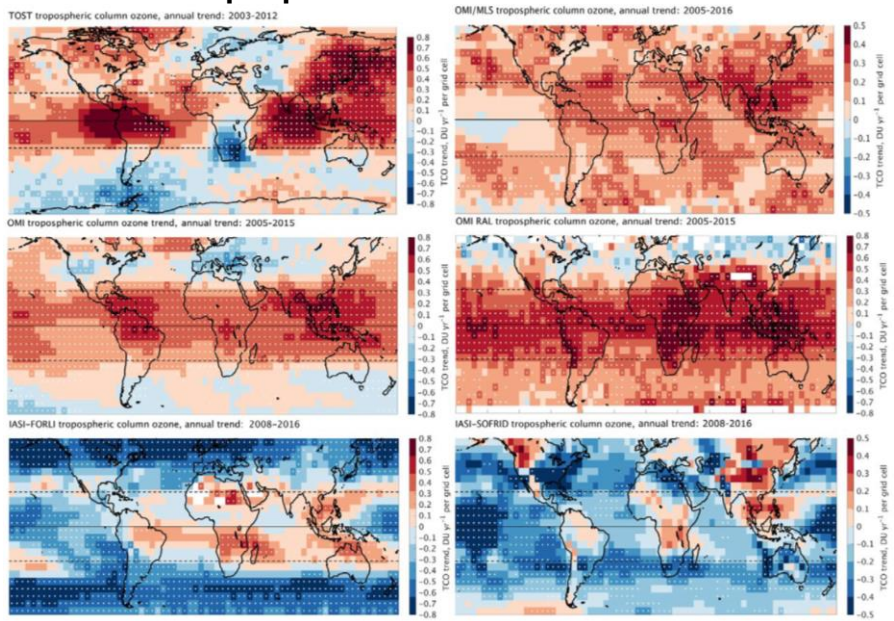
- **TOAR-II Satellite Ozone Working Group**
- **Address above issues**
- **Reconcile satellite-, ground- and aircraft-based data**
- **Global chemistry transport models as transfer standard**
- **Provide common methodology for validation of trends**

Tropospheric Ozone Burden



TOAR tropospheric ozone assessment report

Tropospheric Ozone Annual Trend

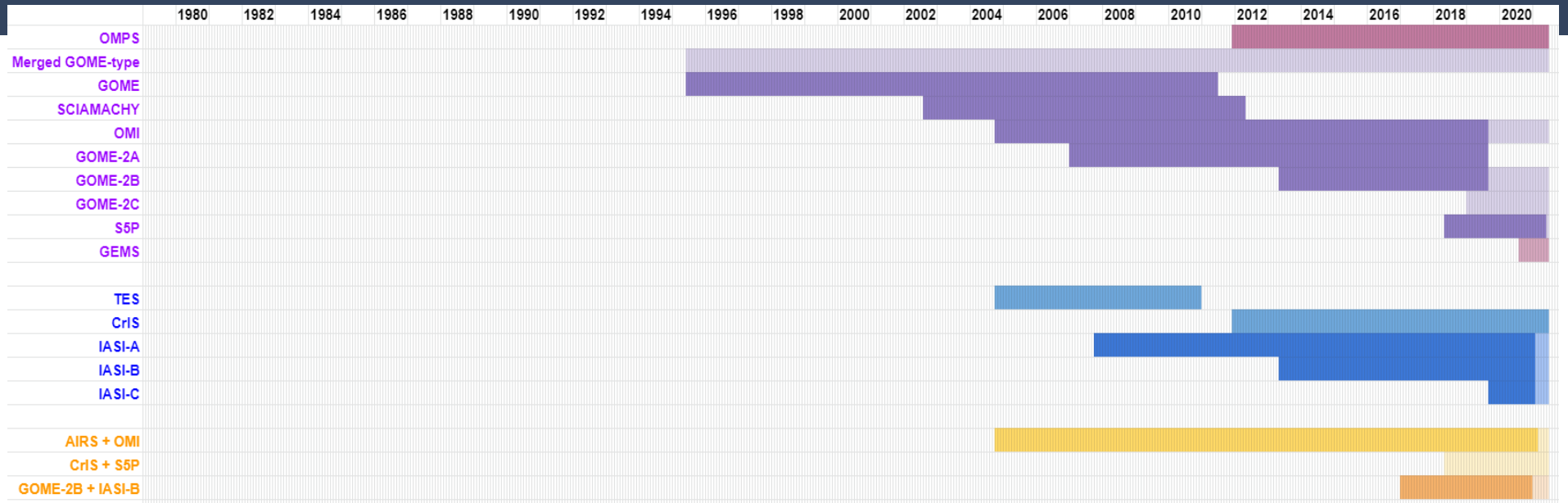


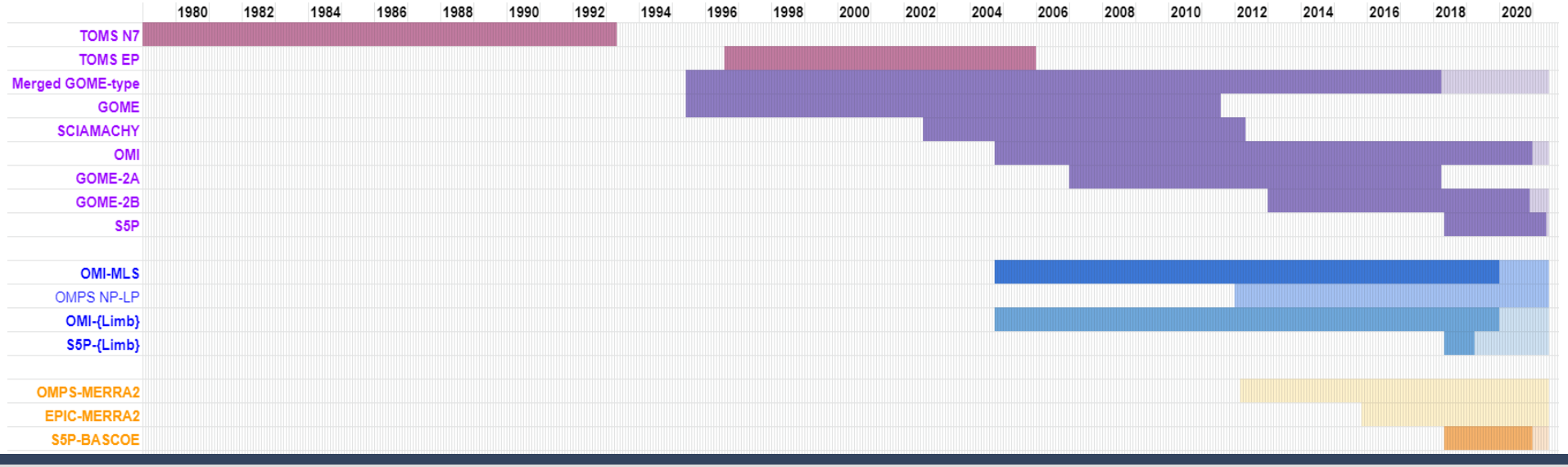
Tropospheric Ozone Validation and Harmonization (2)

VC-20-01	Tropospheric ozone dataset validation and harmonization	2022 Q4	AC-VC

- Coordinator: D. Loyola (DLR)
- Contributors: BIRA-IASB, DLR, ESA, FMI, JPL, KNMI, LISA, NASA, NOAA, RAL, ULB, U.Pusan…
- CEOS response to IGAC TOAR-II needs
- Active cooperation with TOAR-II Satellite Ozone WG and HEGIFTOM WG
- VC-20-01 schedule and status:
  - Kick-off at AC-VC-16 (2020/06), harmonization and validation protocol AC-VC-17 (2021/06)
  - Several TOAR-II SOWG and HEGIFTOM meetings in 2021 and 2022
  - VC-20-01 report at AC-VC-18 (March 2022/03): harmonization and validation results
  - Ongoing: more datasets, further work, scoping of TOAR-II publications (2022+)

Tropospheric Ozone Validation and Harmonization (3)





Optimal Estimation retrieval

→ vertical profile at pixel level or at pixel-cluster level

- UV-VIS
- TIR
- Synergy UV-VIS+TIR

Residual techniques

→ partial column calculated as difference between total and pseudo-stratospheric columns, often gridded in time & space

- Cloud-free TC minus above Convective Cloud TC
- Nadir TC minus Limb PROF
- Nadir TC minus Reanalysis PROF

Tropospheric Ozone Validation and Harmonization (4)

Re-optimized prior matching to common prior constraints

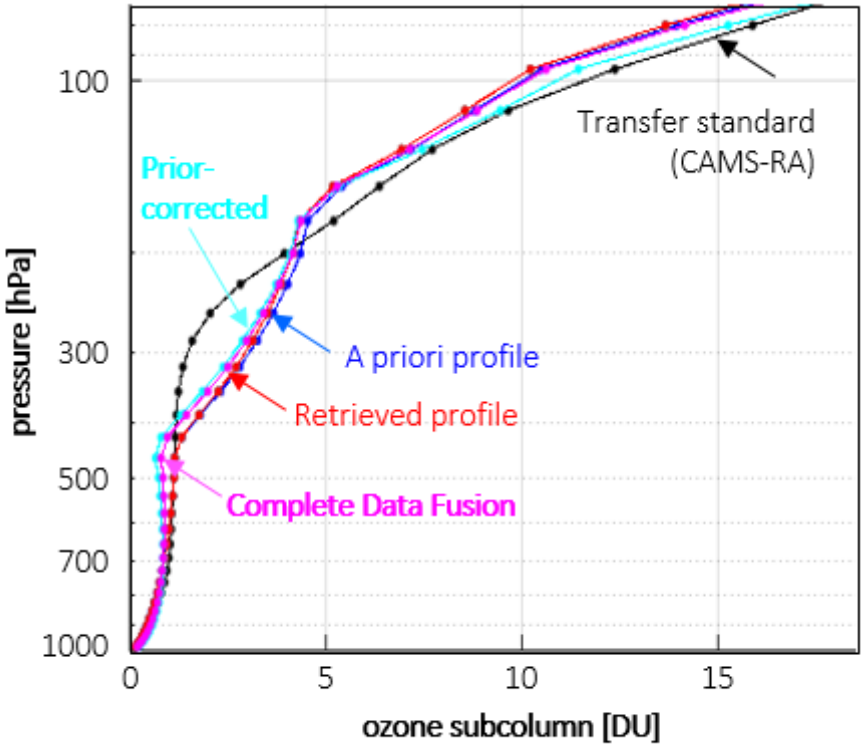
new prior

- Non-optimized prior profile harmonisation:

$$x' = x - (I - A)(x_a - x'_a)$$

- Full prior/smoothing harmonisation using Wiener deconvolution and Complete Data Fusion:

$$x' = (A^T S_x^{-1} A + S_a'^{-1})^{-1} \times (A^T S_x^{-1}(x - (I - A)x_a) + S_a'^{-1} x'_a)$$



Details in:

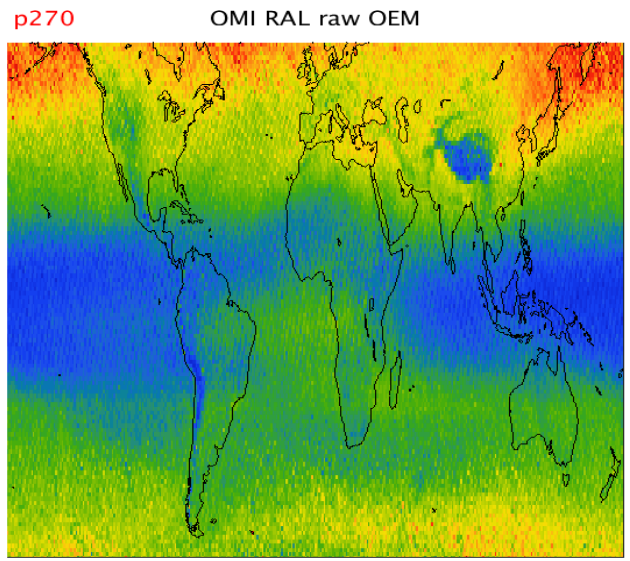
- Evaluation of harmonization methods: Keppens *et al.*, Atmos. Meas. Tech. (2019) https://doi.org/10.5194/amt-12-4379-2019
- CDF removal of prior information: Keppens *et al.*, Remote Sens. (2022) https://doi.org/10.3390/rs14092197

Courtesy A. Keppens et al. (BIRA-IASB)

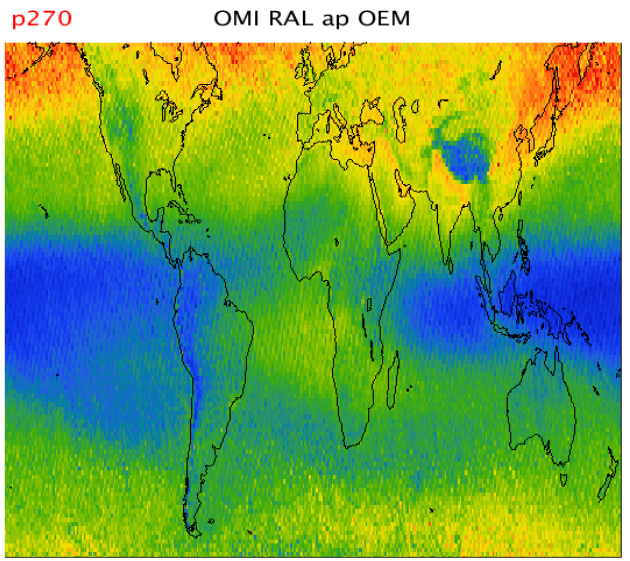
Tropospheric Ozone Data Harmonization

Example: OMI RAL O3 Profile 2016-2018

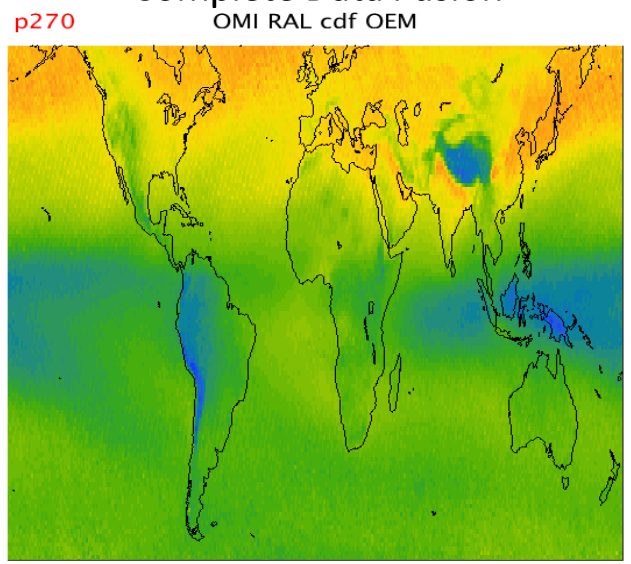
Retrieved

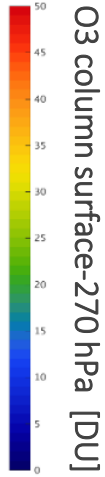


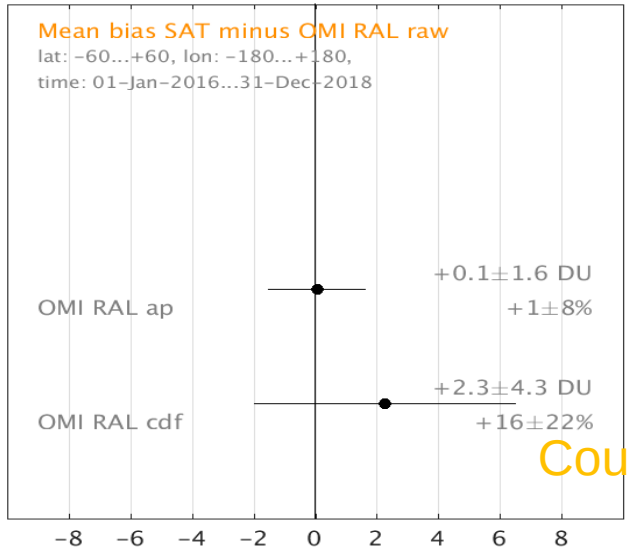
Prior corrected

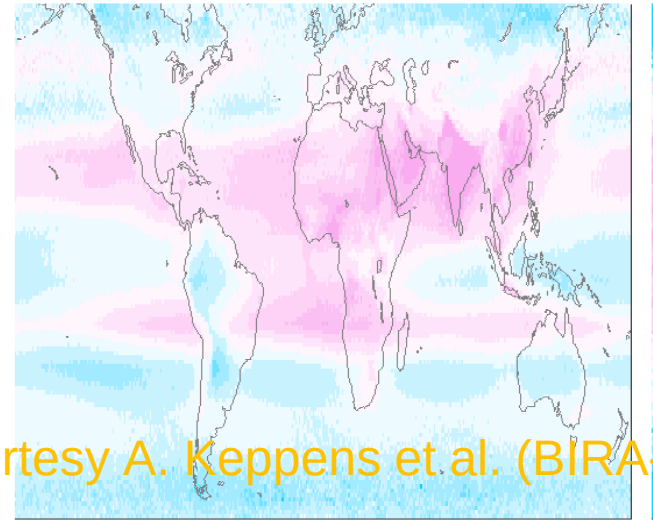


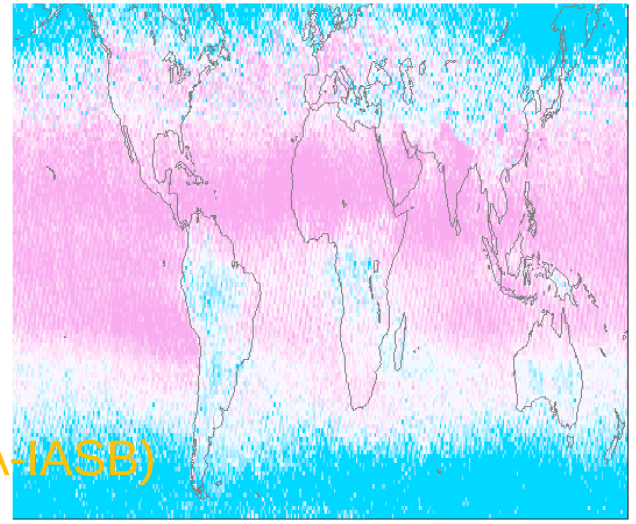
Complete Data Fusion











Courtesy A. Keppens et al. (BIRA-IASB)

Tropospheric Ozone Validation and Harmonization (6)

before harmonization of top level

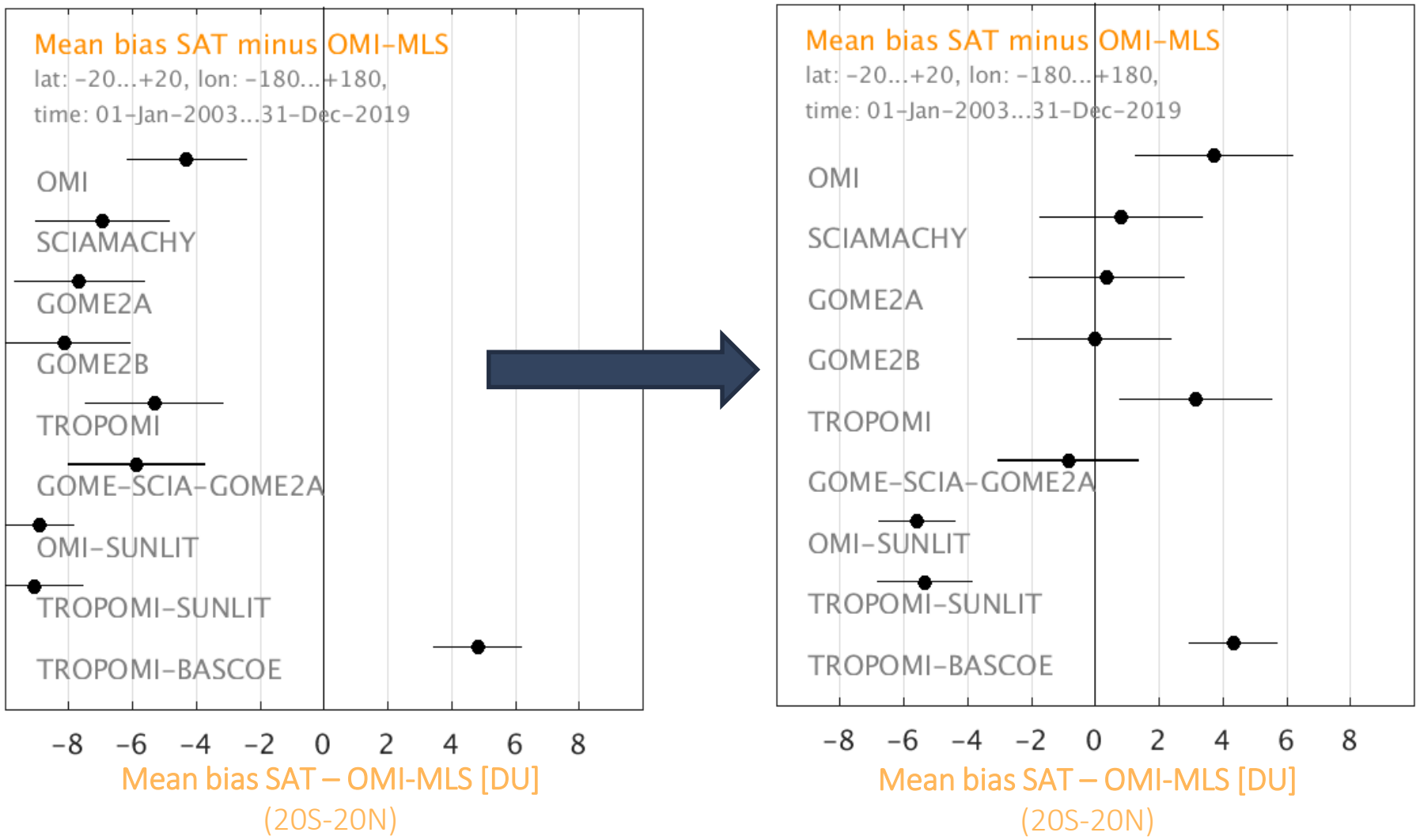
after harmonization of top level

270 hPa

200 hPa

lapse rate TP – 3 km

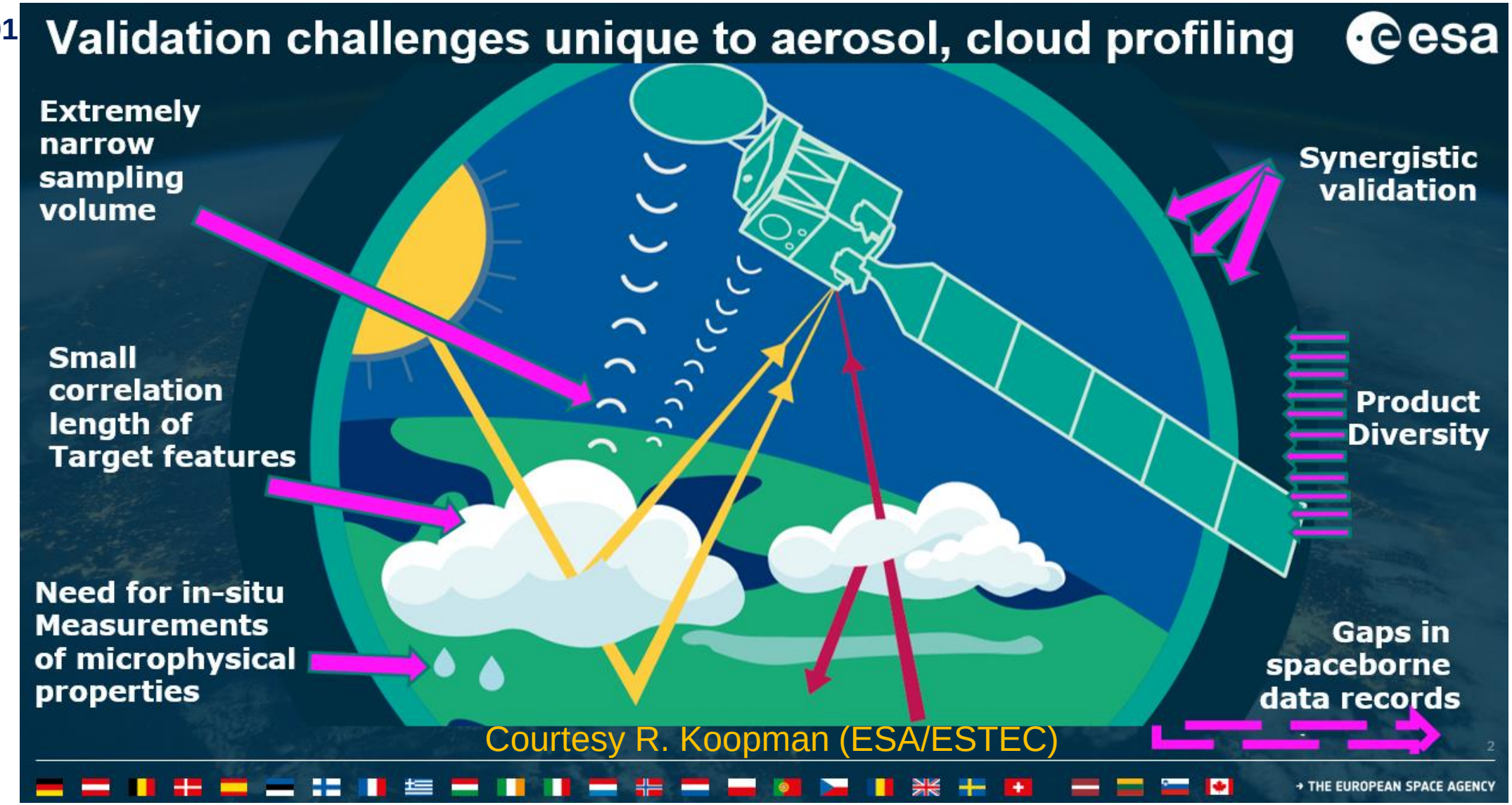
dynamical TP



Courtesy D. Hubert et al. (BIRA-IASB)

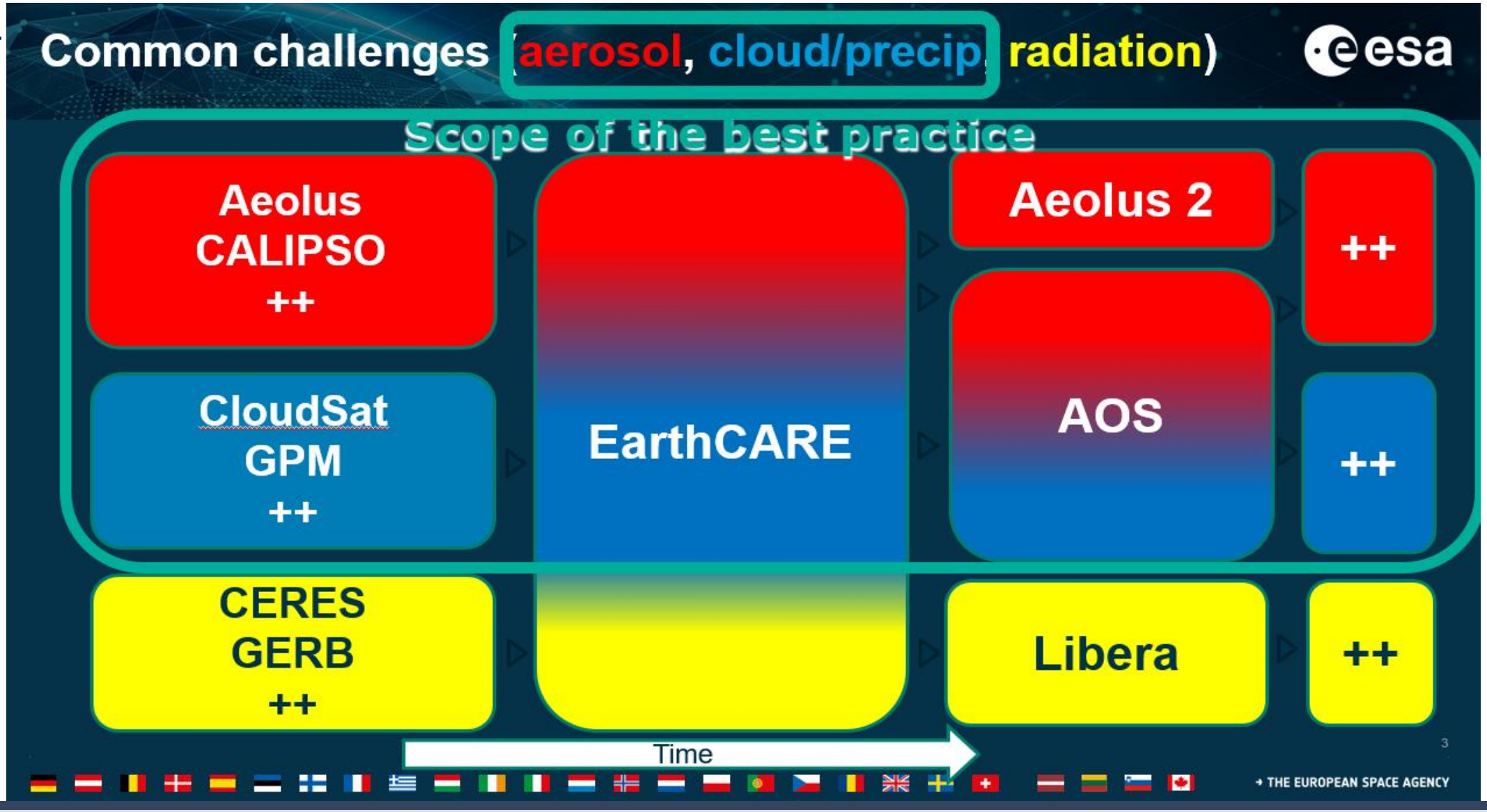
Validation protocols for aerosol and cloud profiles (1)

CV-22-01



Validation protocols for aerosol and cloud profiles (2)

CV-22-01



Validation protocols for aerosol and cloud profiles (3)

CV-22-01

Primary benefit

esa

Improved data quality from upcoming EO missions

- Knowledge transfer and exchange:
  - Between successive missions ("*pensioner to postdoc*")
  - Between correlative instrument providers and validation teams
  - Between algorithm developers and validation teams
- Optimised/harmonised (super)site equipment (serving multiple missions)
- Global network of networks, in terms of correlative data QA/QC
- Disambiguation of validation results/interpretation from different teams
- Improving data record continuity (e.g. handling of wavelength differences)
- Python code for broader community, easily adaptable to multiple missions, under permissive open source licence (compliant with NASA-ESA Multi-Mission Algorithm and Analysis Platform)

4

→ THE EUROPEAN SPACE AGENCY

Validation protocols for aerosol and cloud profiles (4)

CV-22-01

Status

- High-resolution profile validation of aersol, cloud, and precipitation is challenging
- A need for intense community exchange on methods and approaches has been identified
- Initial thoughts on how to achieve this have been exchanged with a few participants from the AOS and EarthCARE 2021 workshops. Present approach is a self-organised community model, fostered and supported by space agencies.
- Athough the bulk of the work remains voluntary (hence the idea to also publish the work in peer-reviewed journal), ESA has foreseen a contribution to some of key scientists on the EarthCARE side that will engage the broader community, and to developers of the open source tools implementing suborbital-to-orbital transformation best practices: the development of suborbital-to-orbital transformation tools for lidar and imagers is already underway.
- The NASA AOS Sub Orbital Working Group expressed its agreement and would like to participate and could see the value and interest in other AOS groups (instrument teams, algorithm teams, etc.) also participating.
- JAXA participates as observer

5

→ THE EUROPEAN SPACE AGENCY

Validation protocols for aerosol and cloud profiles (5)

CV-22-01