living planet symposium | BONN 23–27 May 2022

TAKING THE PULSE OF OUR PLANET FROM SPACE

APPROACH TO ALTIUS OZONE PROFILE VALIDATION

Jean-Christopher Lambert, Daan Hubert, Steven Compernolle, Quentin Errera, José Granville, Tijl Verhoelst, Bjorn Frommknecht, Rob Koopman, Daniel Navarro-Reyes, and Claus Zehner

23 May 2022

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Approach to ALTIUS Ozone Profile Validation

1. ALTIUS mission requirements
2. Validation means
3. Heritage systems
4. Phase E1 planning

Scope of ALTIUS Ozone Data Validation

Mission and User Requirements

- ALTIUS Mission Requirement Document (MRD)
- Earth Watch mission ⟶ user-oriented operational solution

- OPEROZ report
- GCOS Implementation Plan
- CEOS AC-VC interoperability requirements
- Other sources identified

Mission requirement (target / threshold)	Near-real-time (ALT-MRD-PRI-010)	Ozone climatologies (ALT-MRD-PRI-020)	Ozone hole (ALT-MRD-PRI-010)
Altitude range [km]	15-45	20-45	15-45
Vertical resolution [km]*	0.5 / 1	0.5 / 1	1 / 2
Across-track resolution [km]	50 / 100	50 / 100	20 / 100
Along-track sampling [km]	200	200	N.A.
Geographical coverage	global	global	polar
Uncertainty [ppbv]	50 / 100	50 / 100	50 / 100
Uncertainty [%]	5 / 20	3 / 10	10 / 30
Data latency	< 3 hours	4 weeks	4 weeks

Mission requirement (target values)	Mesospheric ozone (ALT-MRD-SEC-010)	3-D tomographic ozone fields (ALT-MRD-SEC-120)
Altitude range [km]	45-100	15-45
Vertical resolution [km]*	1	1
Across-track resolution [km]	50	2
Along-track sampling [km]	200	200
Uncertainty [%]	10	5

* Resolution requirements are currently under discussion.

Requirement	Middle and lower stratosphere	Upper stratosphere and mesosphere
Frequency	4 hours	daily
Vertical resolution [km]	2	3
Horizontal resolution [km]	200	200
Measurement uncertainty [%]	10	5-20%
Stability per decade [%]	2	2

Specific Level-2 validation targets

- Validation of geophysical quantity value with production of diagnostic (ex-post) uncertainty estimates
- Validation of prognostic (ex-ante) uncertainty estimates
- Dependence on influence quantities
- Analysis of retrieval diagnostics
- Verification of data Quality Flags

Table 8 – Specific requirements for ALTIUS Level-2 ozone profile data validation. Observation modes: BL = Bright Limb, SO =Solar Occultation, ST = Stellar Occultation.

Variable	ALTIUS mode BL	SO	ST	Range	Rationale
Ozone density:					
15-20 km (UTLS)	X	X	X	1-3 10^{12} molec.cm^{-3}	Measurand
20-35 km (MS)	X	X	X	2-7 10^{12} molec.cm^{-3}	
35-45 km (US)	X	X	X	0.1-1.5 10^{12} molec.cm^{-3}	
Influence quantity	**BL**	**SO**	**ST**	**Range**	**Rationale**
Temperature	X	X	X	0-50 km profile 180 K (O_3 hole) to 290 K	Major influence quantity, unit conversion
Pressure	X	X	X	0-50 km	Scattering, altitude registration, unit conversion
Cloud top height	X	X	X		Boundary, upwelling radiation
Cloud top albedo	X	X	X		Upwelling radiation
Aerosol height	X	X	X		Boundary, upwelling radiation
Surface albedo	X	X	X	0.05 (ocean) to 0.95 (ice)	Upwelling radiation
Star temperature			X X	2300 K to 7000 K (cool) 7000 K to 46,000 K (hot)	Signal-to-noise ratio
Star magnitude			X	-2 (strong) to +4 (weak)	Signal-to-noise ratio
Solar zenith angle	X 	 X 	 X	0° - 90° 90° - 108° 108° - 180°	Identifies radiation source, controls radiative transfer
LOS azimuth angle			X X X	-10° to 10° (back) +10° to +45° (slant) +45° to +90° (side)	Identifies radiation source, controls radiative transfer, determines profile geometry
Obliquity, beta angle		X	X		Determines sensing conditions and resolution
Occultation type		X	X	Rise, set at spacecraft Rise, set at tangent point	Diurnal cycle
Diagnostics	**BL**	**SO**	**ST**	**Range**	**Rationale**
Quality flags	X	X	X	For each level and profile	Removal of outliers
Vertical averaging kernel matrix (AK)	X	X	X	Ideally for each retrieval; or at minimum 1 representative matrix per observation mode, latitude zone, month…	Required for information content studies, DFS, vertical resolution, altitude registration…
Error covariance matrix (ECM) or error profile	X	X	X	Ideally for each retrieval; or at minimum 1 representative matrix per observation mode, latitude zone, month…	Significance of (dis)agreement with correlative measurements, validation of reported errors
Chi-square, RMS	X	X	X	With every ozone value / retrieval	Quality indicator for retrieval

ALTIUS Validation Approach

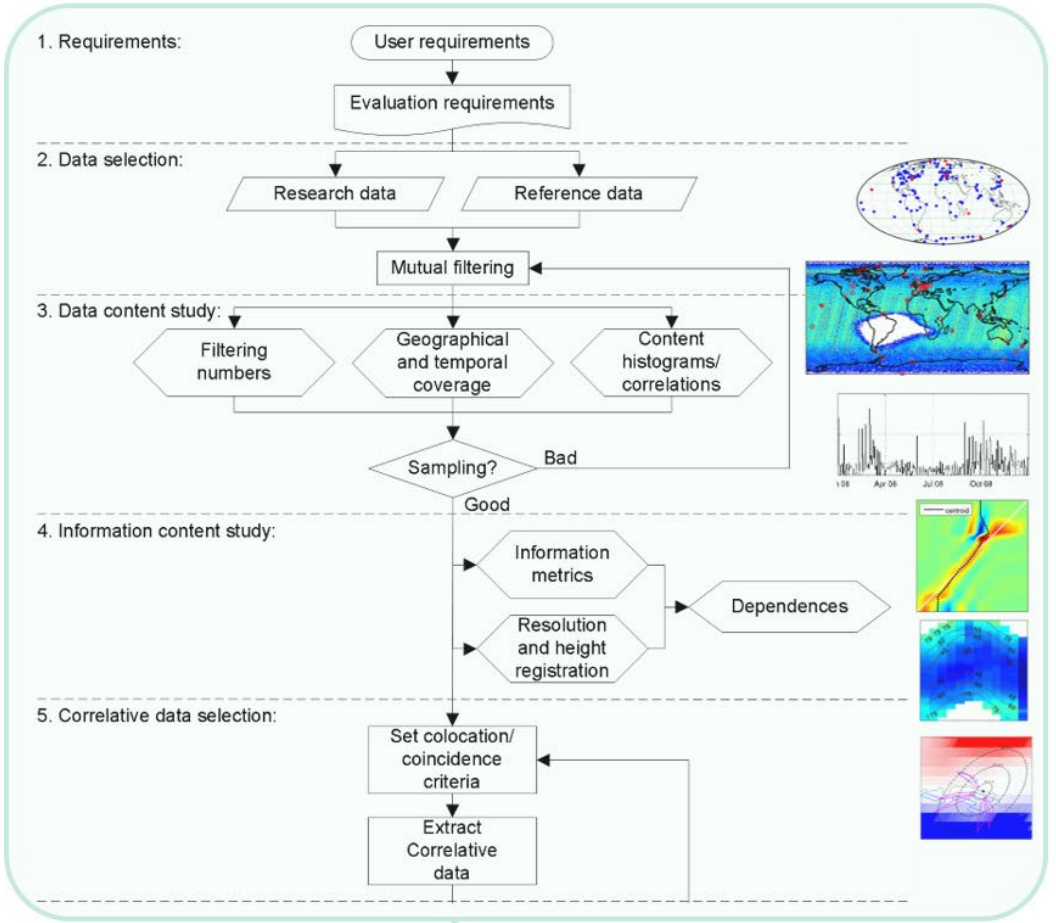
45 requirements

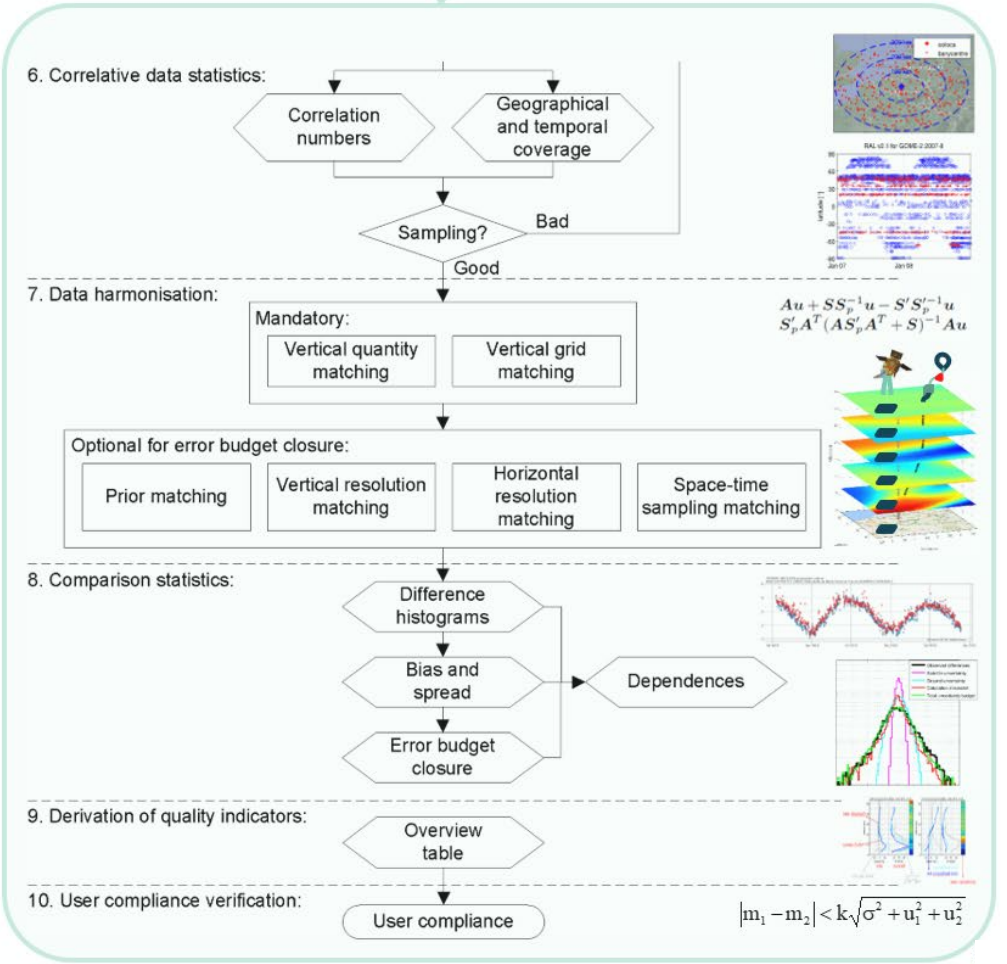
- Standards
- Cardinal validation targets
- Mission and user requirements
- Data content and documentation
- Validation approaches
- Data analysis
- Planning and organization
- Tools and services

Identifier	ALTIUS validation requirement by category	Sections
STANDARDS AND TRACEABILITY		
ALT-CV-REQ-001	ALTIUS Cal/Val activities shall adhere to the general EO data quality strategy established in the QA4EO framework.	4.1
ALT-CV-REQ-002	Traceable Quality Indicators shall be produced to enable users to evaluate readily the fitness-for-purpose of the ALTIUS data.	4.1
ALT-CV-REQ-003	ALTIUS Cal/Val activities shall adopt standards and best practices for terminology.	4.1, 2.3, 2.4
ALT-CV-REQ-004	ALTIUS Cal/Val activities based on data comparisons shall adopt a community endorsed process of generic validation operations.	4.4
ALT-CV-REQ-005	Maturity of the ALTIUS Cal/Val shall be assessed at minimum against the CEOS WGISS Data Management and Stewardship Maturity Matrix for satellite data validation.	4.5
ALT-CV-REQ-006	Traceability of the ALTIUS validation process, methods, tools and data shall be documented.	4.1
ALT-CV-REQ-007	Validation reporting shall include traceability information on the ALTIUS data product, the validation processing, and the validation team(s) issuing the report.	4.1
CARDINAL VALIDATION TARGETS		
ALT-CV-REQ-008	Quality indicators shall be established for Level-2 geophysical quantities (vertical profile of ozone concentration).	4.1, 4.2, 4.3.8, 5.1
ALT-CV-REQ-009	Validity of the ancillary and auxiliary parameters used by the Level-1-to-2 data processors shall be verified.	4.2, 5.1
ALT-CV-REQ-010	Theoretical ex-ante uncertainties associated with the Level-1b and Level-2 data products shall be given quantitative evidence of their validity.	4.2, 4.3.8, 5.1
ALT-CV-REQ-011	Quality flags and of data usage recommendations associated with the data products shall be given evidence of their validity and efficiency.	4.2, 5.1
ALT-CV-REQ-012	Compliance of actual quality of the data product shall be evaluated with respect to mission requirements and core user requirements.	4.2, 5.1
ALT-CV-REQ-013	Compliance of actual quality of the data product shall be evaluated with respect to product specifications.	4.2, 5.1
MISSION AND USER REQUIREMENTS		
ALT-CV-REQ-014	Cal/Val activities shall establish quality indicators enabling to judge the fitness-for-purpose of the ALTIUS data quality comply with product specifications and mission requirements.	3.2, 3.3

Generic Ozone Profile Validation Protocol

(provides Quality Indicators, includes round-robin function)



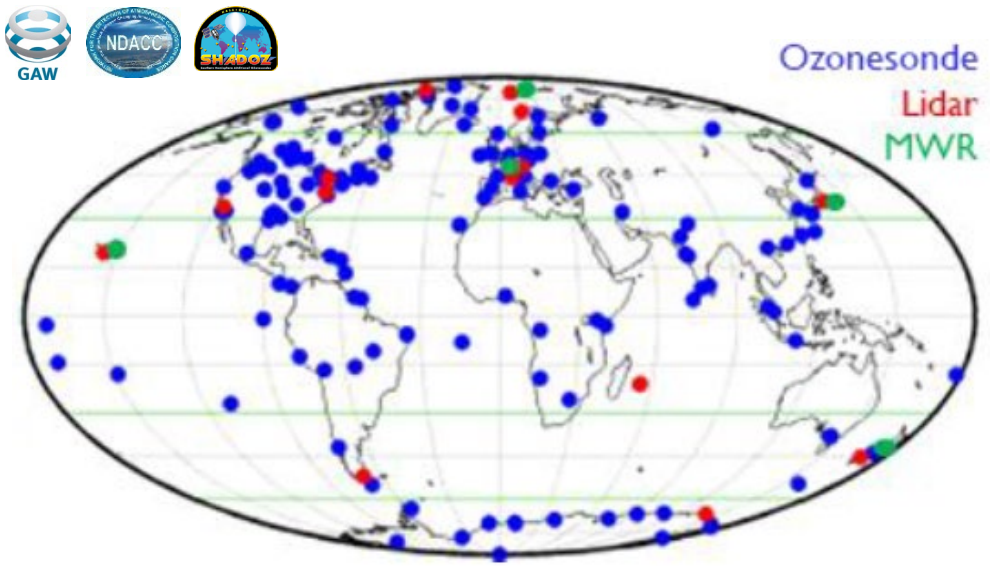


Keppens *et al.*, AMT 2015

Comparisons to ground-based monitoring networks

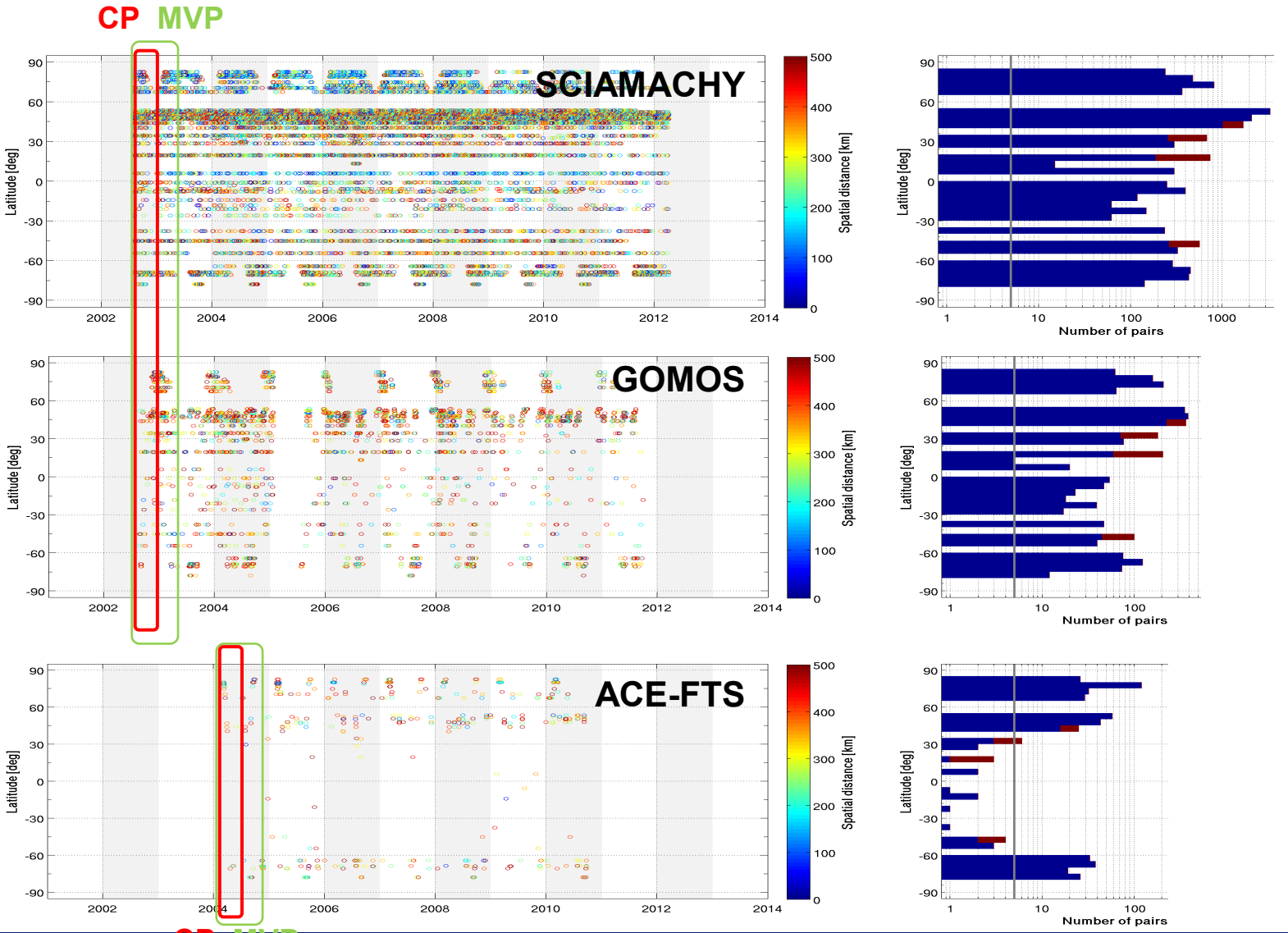
Table 9 – Ground-based capabilities envisaged for ALTIUS Level-2 ozone profile validation during Phase E1.

Instrument	Altitude / vert. resolution	Local time	Uncertainty	Comments / Priority
Balloon-borne electrochemical ozonesonde	ground → 30 km / 150 m	mostly daytime, all weather	5%	Best vertical resolution, worldwide coverage / first priority
Differential Absorption Lidar (DIAL)	15 → 50 km / 0.5 km @ 15 km 7 km @ 50 km	night-time, clear weather	2% @ 15-35 km 5-20% @ 35-50 km	Good vertical resolution and stratospheric range, limited geographical coverage, clear weather night-time only / first priority
Millimetre Wave Radiometer (MWR)	20 → 65 km / 8 km @ 20-40 km 19 km @ 60 km	day and night, all weather	6-9% @ 20-54 km 11% @ 64 km	Low vertical resolution and poor geographical coverage, but very dense day-and-night coverage, demonstrated for trend studies / mid-term priority, high priority for mesospheric ozone



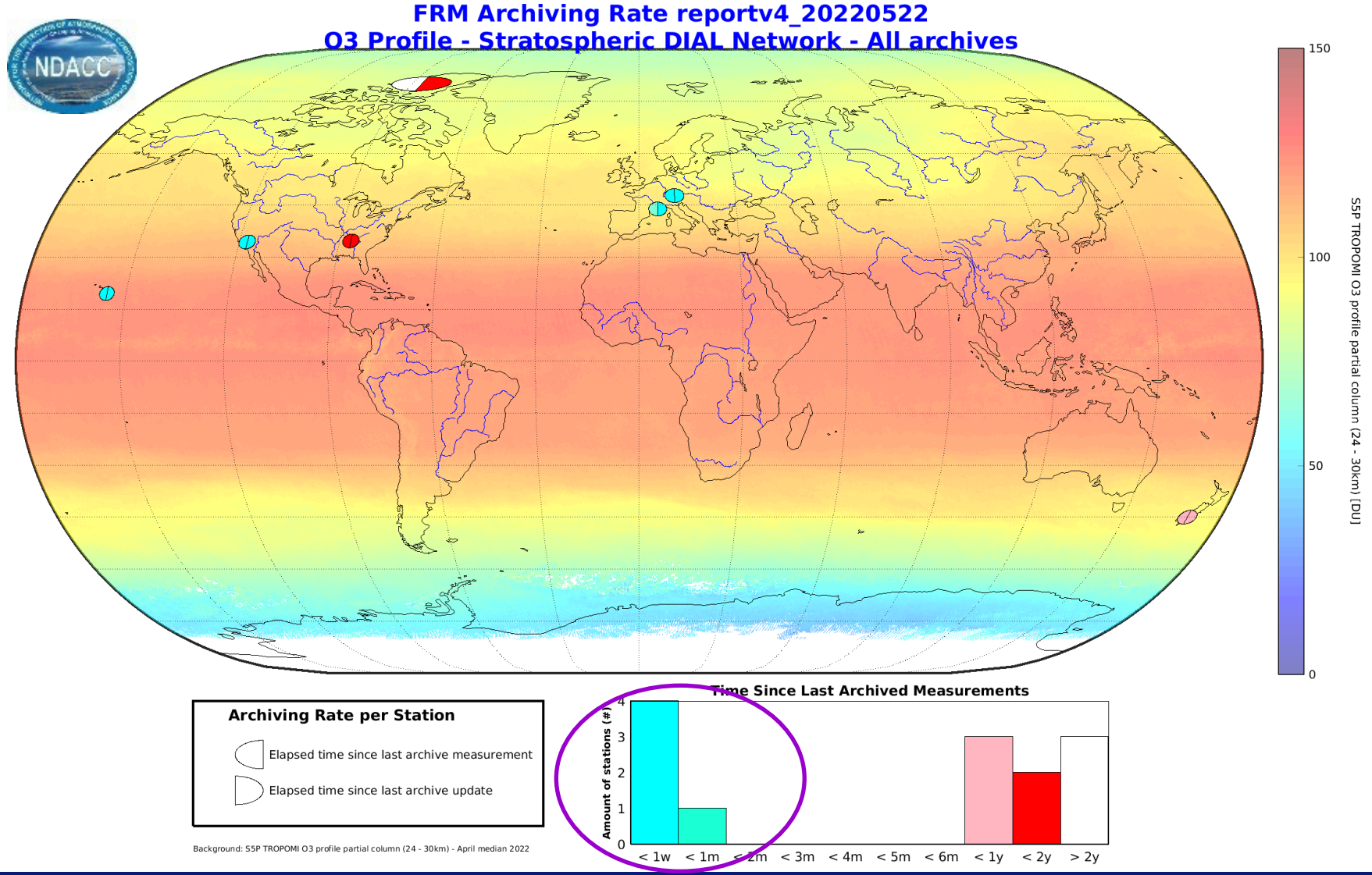
Comparisons to ground-based monitoring networks

Co-locations with historical Limb, Stellar and Solar occultation sounders



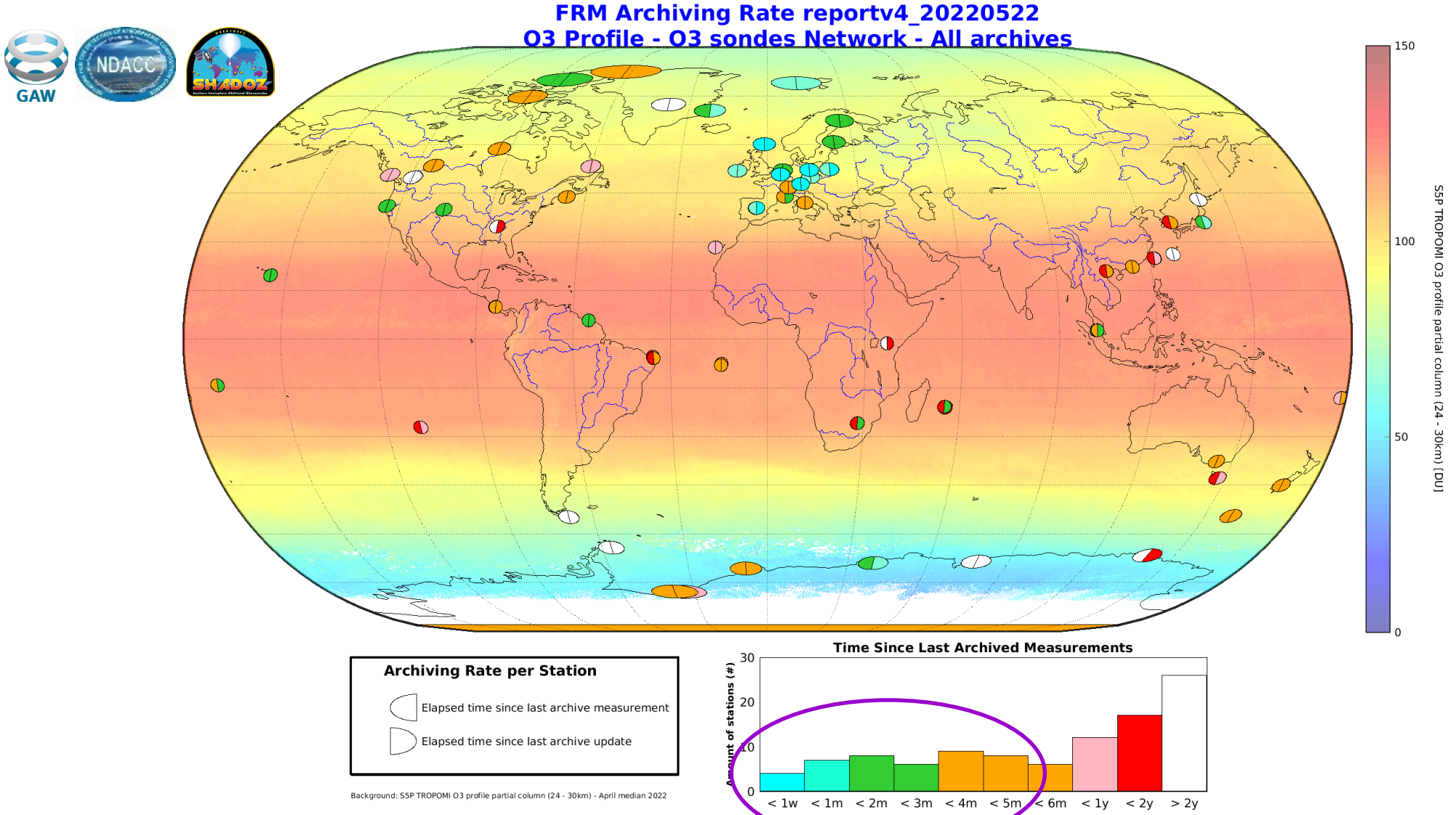
Comparisons to ground-based monitoring networks

Timeliness of NDACC Lidar data availability over the last 2 years



Comparisons to ground-based monitoring networks

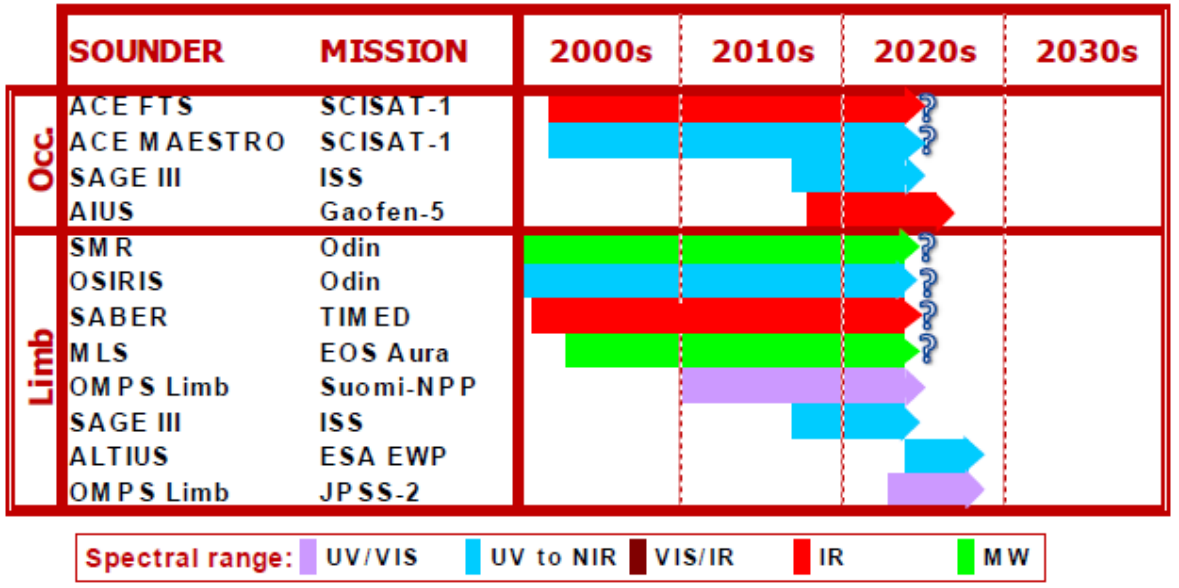
Timeliness of ozonesonde data availability over the last 2 years

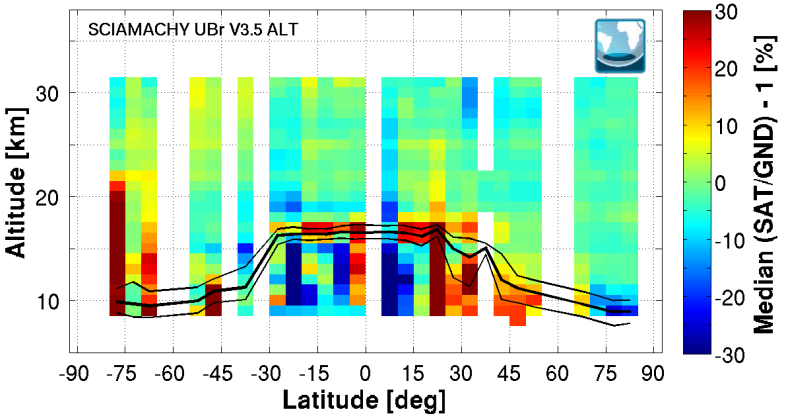


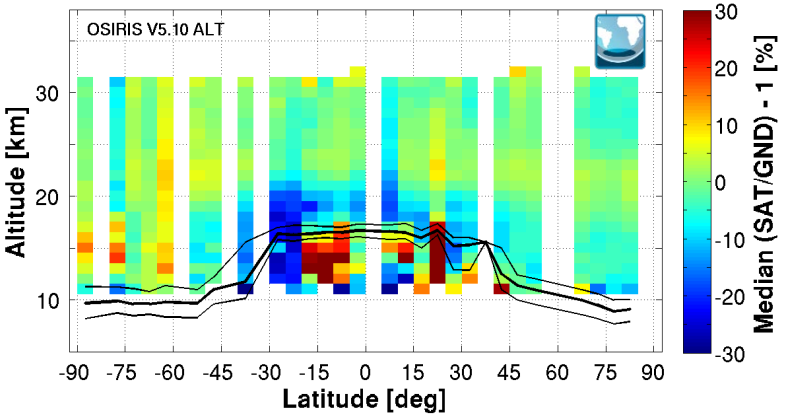
Cross-validation with other satellites

Comparison with Limb, Solar occultation and Nadir sounders

- Several approaches, including comparisons of pairs, of zonal means, and using ground-based network data as a transfer standard
- Detection of features not accessible from the ground and by point-like FRMs
- Compliance with CEOS interoperability requirements
- Cross-validation with alternative ALTIUS L2 retrievals

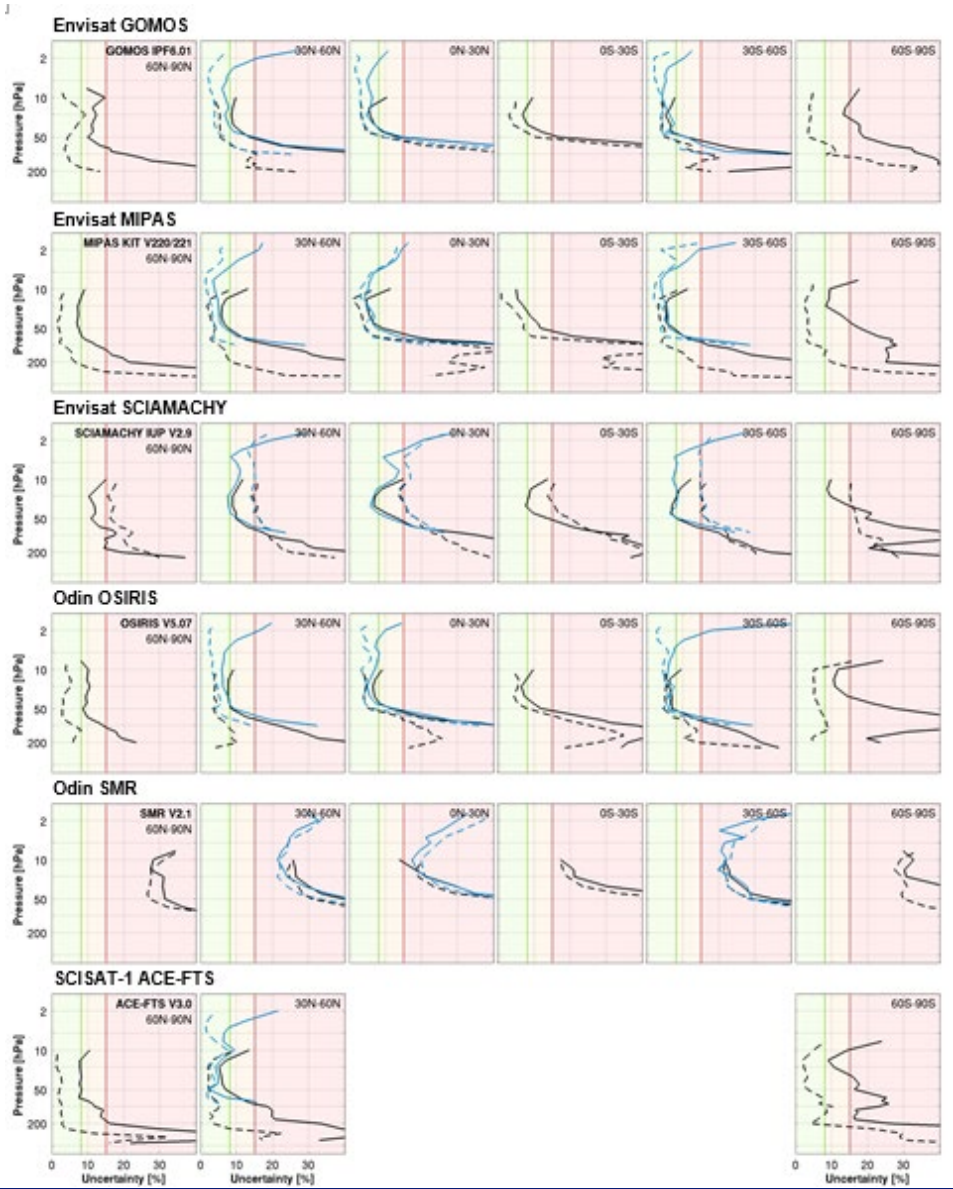






Cross-validation with other satellites

- Compliance with GCOS & Ozone_cci+ CRG requirements
- Compliance with CEOS interoperability requirements

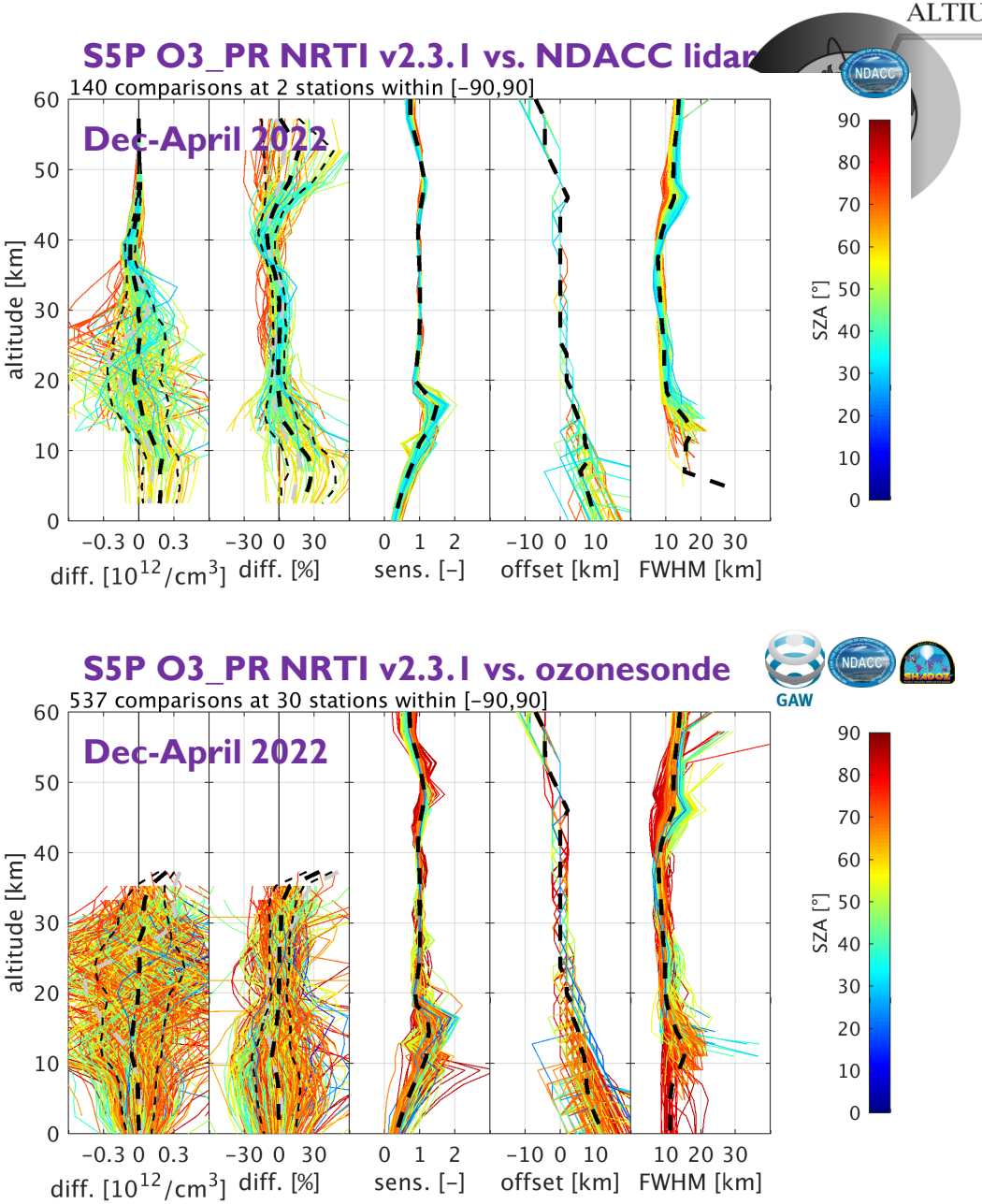


Analysis of information content and other diagnostics

Combination of data comparisons and of information content analysis

Example: Sentinel-5p TROPOMI ozone profile validation:

- DFS ~ 6 pieces of independent information
- Sensitivity ~0.5 at surface, ~1.5 peak in UTLS
- Vertical resolution ~10-15 km, 7 km @ 35 km
- Altitude registration ~-10 km offset (towards surface) in troposphere, max. +2 km offset in middle stratosphere
- Increased sensitivity and better resolution at high SZA
- Data outliers over high surface albedo



Courtesy A. Keppens *et al.* (BIRA-IASB, S5P MPC)

Modelling support

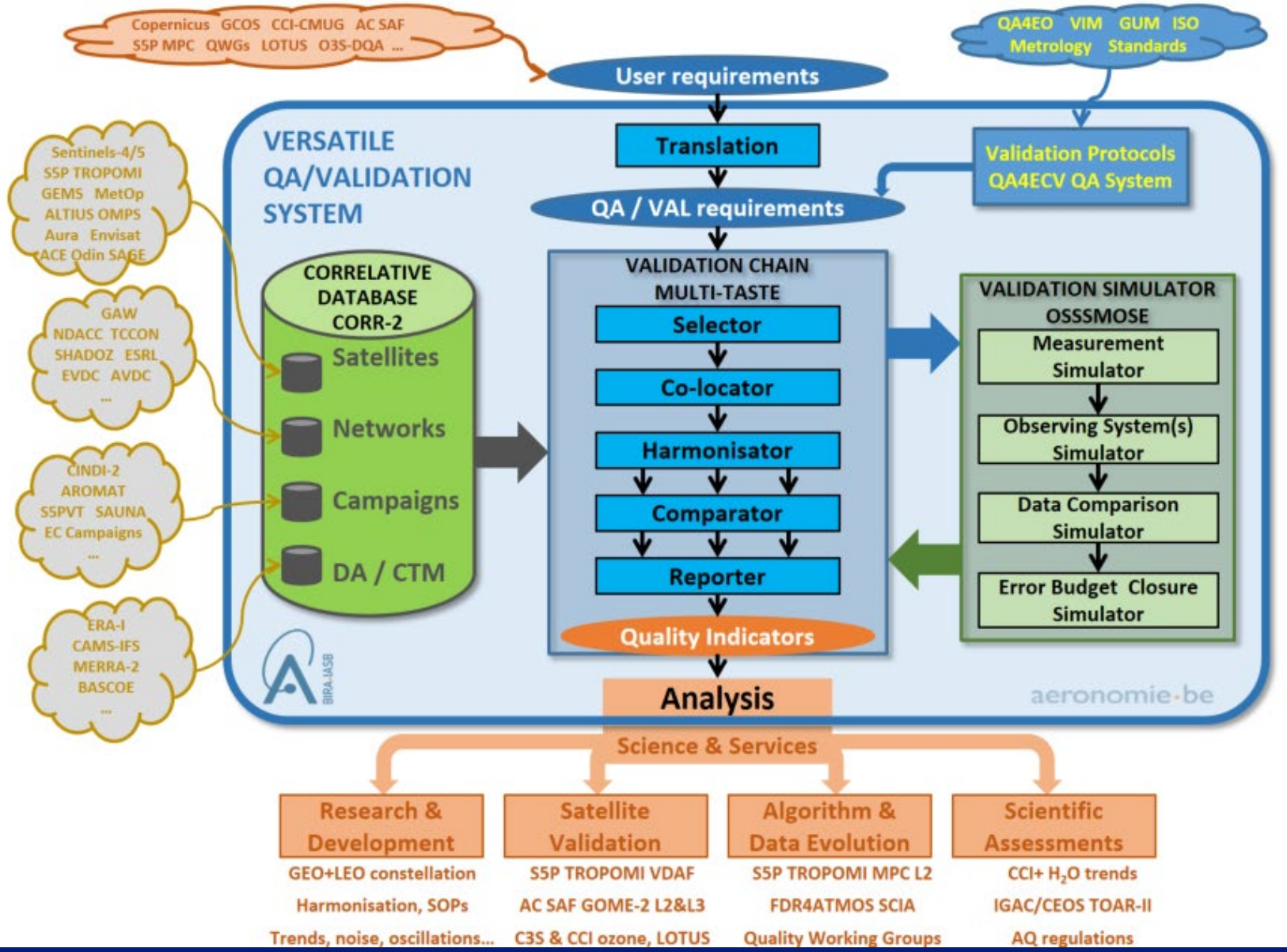
Early involvement of BASCOE 4D-var data assimilation system (Belgium), ECCC (Canada) modelling, and ECMWF (CAMS-IFS), preferably in parallel to FRM-based comparisons and satellite cross-validation:

- to get complementary insight into ALTIUS data quality
- to detect features not accessible by data comparisons
- to assess ALTIUS products readiness for data assimilation and applications.

Assessment of co-location mismatch uncertainties and of their impact on comparison results using metrology simulator OSSSMOSE

Multi-TASTE :

Multi-platform QA/Validation Expert System

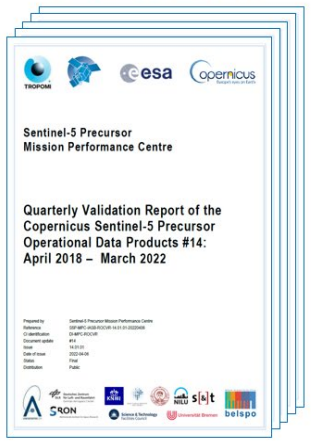


Pathfinder: the ESA/Copernicus Sentinel-5p MPC Routine Operations Validation Service

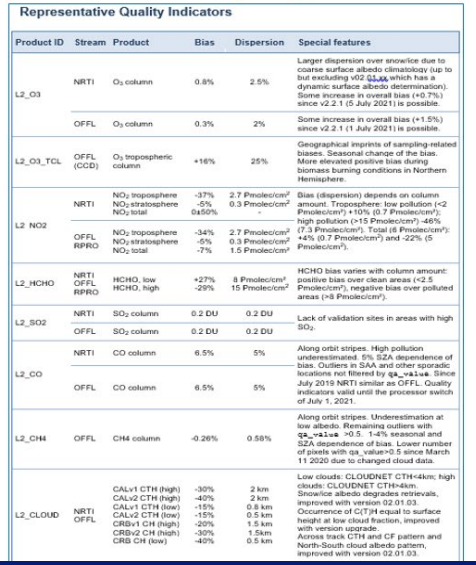
- **Monitoring of** S5P products **health**
- Maintenance of S5P data quality **documentation**
- **In-depth validation** and support to L1/L2 **algorithm evolution**
- Synthesis with **S5PVT** results, **ECMWF/CAMS**, peer-reviewed literature…

Routine Operations Validation Platform http://mpc-vdaf.tropomi.eu

Quarterly Validation Report



Maintenance of Quality Indicators



Representative Quality Indicators

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 surface albedo determination). Some increase in overall bias (+0.7%) since v2.2.1 (5 July 2021) is possible.
	OFFL	O_3 column	0.3%	2%	Some increase in overall bias (+1.5%) since v2.2.1 (1 July 2021) is possible.
L2_O3_TCL	OFFL (CCD)	O_3 tropospheric column	+16%	25%	Geographical imprints of sampling-related biases. Seasonal change of the bias. More elevated positive bias during biomass burning conditions in Northern Hemisphere.
L2_NO2	NRTI	NO_2 troposphere NO_2 stratosphere NO_2 total	-37% -5% 0±50%	2.7 Pmolec/cm² 0.3 Pmolec/cm² -	Bias (dispersion) depends on column amount. Troposphere: low pollution (<2 Pmolec/cm²) +10% (0.7 Pmolec/cm²); high pollution (>15 Pmolec/cm²) -46% (7.3 Pmolec/cm²). Total (8 Pmolec/cm²): +4% (0.7 Pmolec/cm²) and -22% (5 Pmolec/cm²).
	OFFL RPRO	NO_2 troposphere NO_2 stratosphere NO_2 total	-34% -5% -7%	2.7 Pmolec/cm² 0.3 Pmolec/cm² 1.5 Pmolec/cm²	
L2_HCHO	NRTI OFFL RPRO	HCHO, low HCHO, high	+27% -29%	8 Pmolec/cm² 15 Pmolec/cm²	HCHO bias varies with column amount: positive bias over clean areas (<2.5 Pmolec/cm²), negative bias over polluted areas (>8 Pmolec/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. Quality indicators valid until the processor switch of July 1, 2021.
	OFFL	CO column	6.5%	5%	
L2_CH4	OFFL	CH4 column	-0.26%	0.58%	Along orbit stripes. Underestimation at low albedo. Remaining outliers with qa_value >0.5. 1-4% seasonal and SZA dependence of bias. Lower number of pixels with qa_value>0.5 since March 11 2020 due to changed cloud data.
L2_CLOUD	NRTI OFFL	CALv1 CTH (high) CALv2 CTH (high) CALv1 CTH (low) CALv2 CTH (low) CRBv1 CH (high) CRBv2 CH (high) CRB CH (low)	-30% -40% -15% -15% -20% -30% -40%	2 km 2 km 0.8 km 0.5 km 1.5 km 1.5km 0.5 km	Low clouds: CLOUDNET CTH<4km; high clouds: CLOUDNET CTH>4km; Snow/ice albedo degrades retrievals, improved with version 02.01.03. Occurrence of CTH 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.

Product Readme Files

ALTIUS validation operations and organization – Phase E1

- Mission Performance Cluster (MPC) like organization and facilities recommended
  - Level-1 and Level-2 verification performed by ALTIUS product development and production teams
  - Core validation performed by dedicated VAL team with Multi-TASTE expert toolset
  - Start of validation tasks with the operational validation system that will serve for routine operations validation in Phase E2
  - Close loop between ESA, L1, L2, VAL, core users
- Initial, off-line uptake and assessment of first ALTIUS data by operational user services planning later the assimilation of ALTIUS data in their systems: BASCOE, ECCC, ECMWF (CAMS-IFS)
- Complementary validation activities proposed by external teams responding to an Announcement of Opportunity for ALTIUS validation and coordinated by ESA and partners in the framework of an international ALTIUS Validation Team
- Pre-launch rehearsal campaign(s) required

Future Announcement of Opportunity

- ESA considers publication of an Announcement of Opportunity for the Cal/Val of ALTIUS approximately 2 years before ALTIUS launch.
- Objectives:
  - to open the ALTIUS Cal/Val to the international community and to a wider range of external validation data and activities,
  - to foster exchanges within the validation community and with the instrument and algorithm experts,
  - to address validation of other ALTIUS species than ozone,
  - to promote the use of ALTIUS data.