SPARC TUNER
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Connecting the TUNER framework to Maturity Matrix approaches for satellite data

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TUNER
TOWARDS UNIFIED ERROR REPORTING

ROYAL BELGIAN INSTITUTE FOR SPACE AERONOMY
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Outline

- System Maturity Matrices for atmospheric composition data
- Application to satellite data
- Application to ground-based data
- Connection with SPARC TUNER

Acknowledgment:
ESA/EU Copernicus Sentinel-5 Precursor Mission Performance Centre
ESA CCI+ Precursors

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SMM with relevance to atmospheric composition data: Objectives

- System Maturity Matrix: tool for quality assurance/maturity assessment of
  - Completeness of product: data + uncertainties + flags + documentation (ATBD, PSD…) + …
  - State-of-the-art process, from end to end: use of standards, pre-flight characterization, in-flight calibration, level-1-to-2 retrieval, geophysical validation…
  - Application of FAIR principles: Findable, Accessible, Interoperable, Reusable
- Interoperability:
  - Internal coherence of (institutional) satellite constellations: GHG, AQ, ozone, aerosols…
  - Transparency for information services (e.g., C3S, CAMS, EPA…)
  - Endorsement of Third Party Missions
  - Support and transfer of knowledge to New Space actors
- Maturity level (instead of YES/NO) ⟶ Identification of what could improve

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SMMs with relevance to atmospheric composition data

- EC FP7 CORE-CLIMAX
- ESA CCI

- **CEOS WGISS DMSMM**
- **ESA EDAP**
- WMO SMM DMP

- EC FP7 QA4ECV QA System

Maturity	SOFTWARE READINESS	METADATA	USER DOCUMENTATION	UNCERTAINTY CHARACTERISATION	PUBLIC ACCESS, FEEDBACK, UPDATE	USAGE
1	Conceptual development	None	Limited scientific description of the methodology available from PI	None	Restricted availability from PI	None
2	Research grade code	Research grade	Comprehensive scientific description of the methodology, report on limited validation, and limited product user guide available from PI; paper on methodology is sumitted for peer-review	Standard uncertainty nomenclature is idenitified or defined; limited validation done; limited information on uncertainty available	Data avaliable from PI, feedback through scientific exchange, irregular updates by PI	Research: Benefits for applications identified DSS: Potential benefits identified
3	Research code with partially applied standards; code contains header and comments, and a README file; PI affirms portability, numerical reproducibility and no security problems	Standards defined or identified; sufficient to use and understand the data and extract discovery metadata	**Score 2** + paper on methodology published; comprehensive validation report available from PI and a paper on validation is submitted; comprehensive user guide is available from PI; Limited description of operations concept available from PI	**Score 2** + standard nomenclature applied; validation extended to full product data coverage, comprehensive information on uncertainty available; methods for automated monitoring defined	Data and documentation publically available from PI, feedback through scientifc exchange, irregular updates by PI	Research: Benefits for applications demonstrated. DSS: Use occuring and benefits emerging
4	**Score 3** + draft software installation/user manual available; 3rd party affirms portability and numerical reproducibility; passes data providers security review	**Score 3** + standards systematically applied; meets international standards for the data set; enhanced discovery metadata; limited location level metadata	**Score 3** + comprehensive s description available fro provider; report on inter cor available from PI; paper on v published; user guide availa data provider; comprehe description of operations c available from PI			
5	**Score 4** + operational code following standards, actions to achieve full compliance are defined; software installation/user manual complete; 3rd party installs the code operationally	**Score 4**+ fully compliant with standards; complete discovery metadata; complete location level metadata	**Score 4** + comprehensive s description maintained by provider; report on data ass results exists; user guide is r updated with updates on pro validation; description on p implementation is available f provider			
6	**Score 5** + fully compliant with standards; Turnkey System	**Score 5** + regularly updated	**Score 5** + journal papers on updates are and more compr validation and validatio quantitative uncertainty esti published; operations co regularly updated			

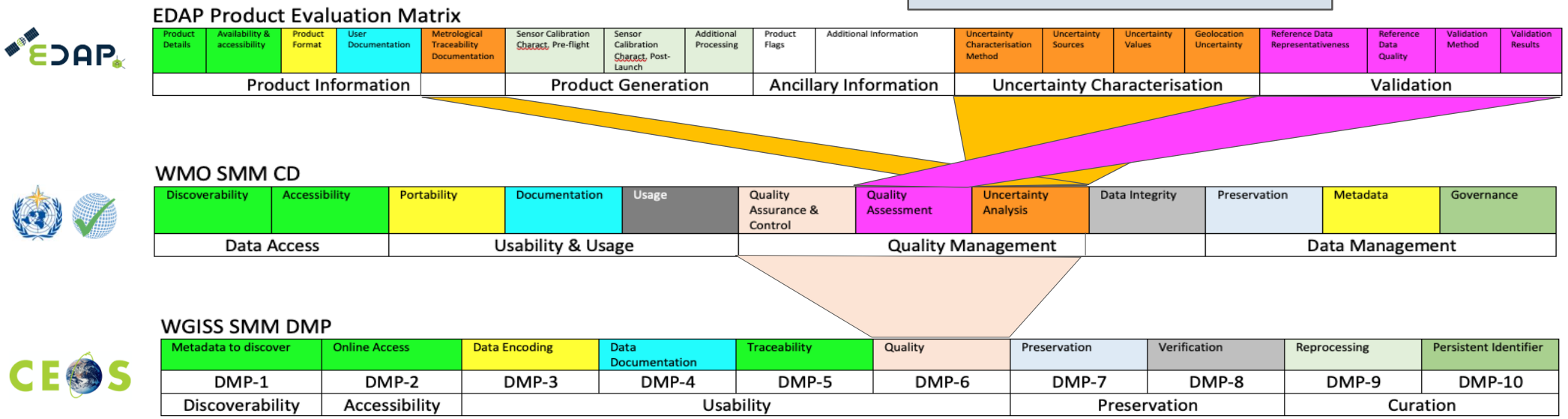
	QA4ECV-Basic	QA4ECV-Intermediate	QA4ECV-Advanced
Details	Documentation available with source code and details on product completeness + consistency	Parameter details provided; ATBD / PUG provides significant detail; forum provided for users	Parameter details split spatially / temporally; ATBD / PUG in line with guidance; forum is monitored
Traceability	High level diagrams with basic information on algorithm provided	Detailed diagrams with relevant sub-chains; detailed information for steps	Detailed information on most steps as well as uncertainty information provided
Flags	Simple flags available in the product with basic information available on derivation and usage	Several flags provided allowing easy distinction of data quality; details provided for each flag	Comprehensive set of flags / ancillary data provided to allow detailed understanding of quality
Validation	Assessed against LPV hierarchy; validation report available and some campaign details	Justification for LPV hierarchy provided; good level of detail provided for validation and intercomparison.	Validation guidance closely followed and comprehensive information on campaigns provided
Uncertainty	Details of uncertainty calculations provided including how they are made available in product and how they should be used	Contributors to uncertainty analysis and calculation details provided with enough information to allow immediate use	Uncertainty significance estimates for all contributors
Assess	Maturity matrix filled in to some extent; GCOS – basic details provided.	All maturity matrix filled in; comments provided for GCOS.	All boxes filled with consensus between producer and auditor.

QA4ECV Help: QA4ECV_helpme@npl.co.uk Version 1.0 – July 2017

Correspondence between SMMs

EDAP vs WMO vs WGISS

The same aspects in the different matrices are identified by the same color



Courtesy Iolanda Maggio (ESA), WGISS-49 (2020/04), https://ceos.org/meetings/wgiss-49/

Take-home message:

- **Data uncertainty**, **QA** and **validation** are recurring themes.
- Different SMM developments correspond to different EO domains and different objectives.
- Harmonization across EO domains and applications → Current SMMs are in evolution.

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WGISS DMSMM

CEOS WGISS Data Management & Stewardship Maturity Matrix

Usability criteria: encoding, documentation, traceability, validation, data uncertainty, QA/QC

not managed

fully managed

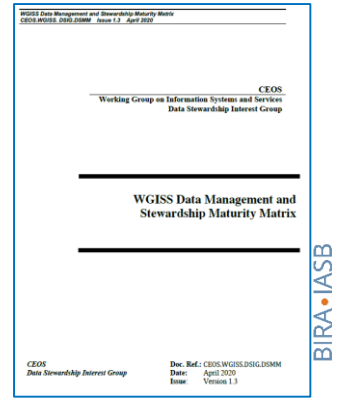
	DISCOVERABILITY	ACCESSIBILITY	USABILITY						PRESERVATION		CURATION	
	MMP1 Metadata for Discovery	MMP2 Online Access	MMP3 Data Encoding	MMP4 Data Documentation	MMP5 Data Traceability	MMP6 Data Validation	MMP7 Data Uncertainty	MMP8 Data Quality Control	MMP9 Data Preservation	MMP10 Data Verification	MMP11 Data Processing/Reprocessing	MMP12 Persistent & Resolvable Identifier
Level-0 Not Managed	1) No catalogue available 2) No advertising available	Data and metadata are not accessible online	1) Data Not Structured 2) Non-standard or proprietary data format, or, poorly-documented standard file format.	Partial and incomplete mission documentation	Limited product information available (not online)	1) Reference Data Representativeness - No validation 2) Reference Data Quality - No validation 3) Validation Method - No validation 4) Validation Results - No validation	1) Uncertainty Method: Uncertainty characterisation not performed, or method not documented. 2) Uncertainty Sources: Uncertainty characterisation not performed, or sources analysed not documented. 3) Uncertainty Values: No uncertainty information provided.	1) No control and monitoring check 2) No quality indicator in metadata 3) No procedures documentation	1) Uncontrolled storage location. 2) Only data are stored 3) Data Records archiving not managed 4) Relevant information on Product Details Assessment not made available	No Data/Associated Information integrity, authenticity and readability check	1) No reprocessing activities planned 2) Pre-flight calibration & characterisation not documented or information not available. 3) Post-launch calibration & characterisation not documented or not available. 4) Processing: Additional processing steps not documented.	No persistent and resolvable identifiers available
Level-1 Partially Managed	1) Advertisi 2) Catalogu available at			1) Already existent		1) Reference Data Representativeness: measurements assessed to be mostly	1) Uncertainty Method: Limited use of				1) Minor updates and bugs corrections of data records implemented	
Level-2 Managed	1) Detailed search avail product lev 2) Product metadata oriented towards an international standard 3) Data Collection and Associated Information searchable. 4) International standard for Collection metadata	Architecture through metadata 2) Data access system oriented towards an international standard	interoperability. 2) Periodically repackaging/ reformatting of archived data. 3) Data in well-documented standard file format, community naming convention standards.	described 2) Link between mission documentation and data records created and managed	correct provenance metadata. Well described product information available online	measurements 2) Reference Data Quality: full uncertainty information 3) Validation Methods assess satellite measurements 4) Validation Results show excellent agreement between satellite and reference measurements, within uncertainties.	separated as Type A or B classification. 2) Uncertainty Sources: All important sources of uncertainty included. 3) Uncertainty Values: Total uncertainty per pixel is provided, with basic breakdown of key components no error-covariance.	1) Quality indicator post-processing available 2) Quality control procedures documented and available online	2) Community-standard for archiving metadata 3) Product Details Assessment: All required information available, any recommended information missing	Information content integrity check and verification 2) Media readability and accessibility testing	reasonable aspects 3) Post-launch calibration & characterisation covers all reasonable aspects of instrument behaviour to a quality that is "fit for purpose" in terms of the mission's stated performance and uses appropriate community infrastructure/methods (CEOS/FRMs). 4) Additional processing steps documented.	Records Collections and metadata 2) Automatic landing page generation and extensive management of landing pages
Level-3 Fully Managed	1) International standard for Product metadata 2) International standard for Collection metadata 3) Catalogue accessible via international or community agreed standards protocol 4) Data policy available in metadata 5) Periodic updates of metadata in the catalogue 6) Quality indicator metadata available and discoverable 7) Search results relevancy. 8) Seamless transition from discovery to access	1) International standard for Data and metadata access system 2) Data policy available in the metadata. 3) Visualisation services 4) Reporting system 5) Hosted processing 6) Quick adoption to new technologies and standards evolution 7) Data and metadata accessible through a free and open access protocol	1) Accepted and Available semantic encoding standards for complete interoperability 2) Data and metadata uses FAIR-compliant vocabularies 3) Analysis Ready Data standard	1) Standards based metadata for documentation 2) Link between mission documentation and data records published	1) Automatic metadata generation for provenance documentation 2) Complete and updated data provenance available online	1) Reference Data Representativeness: Reference measurements independently assessed to be fully representative of the satellite measurements, covering the satellite's full range of measurements and with full assessment of uncertainties and carried out on a regular basis determined by product performance. 2) Reference Data Quality: full uncertainty and error-correlation information, assessed following the GUM and traceable to SI 3) Validation Methods assess satellite measurements and reference data w.r.t. their error- covariance and validates those uncertainties. 4) Validation Results show excellent agreement between satellite and reference measurements, within uncertainties.	1) Uncertainty Method: GUM approach to estimate measurement uncertainty, including a treatment of error-covariance. 2) Uncertainty Sources: All reasonable sources of uncertainty included. 3) Uncertainty Values: Uncertainties per pixel provided with error-covariance information for all appropriate components.	1) Data quality control fully compliant with an international standard 2) Quality indicator pre and post processing available in the metadata 3) Quality metadata assessed	1) Preservation repository officially certified 2) Periodic technology refreshment 3) Identify and manage the basic preservation of relevant mission SW, ensuring that preserved data can be recreated. 4) Continuity of service availability 5) Product Details Assessment: All required and recommended information available	1) Automatic Data Records/Associated Information content integrity check and verification 2) Data authenticity verifiable internally and by the final user 3) Automatic verification process, including monitoring and reporting	1) Reprocessing for time-series creation 2) Roadmap for technology evolution 3) Plurality of accurate and relevant attributes are provided to allow reuse 4) Metadata includes information about the licence 5) Pre-Flight: As Level-2, additionally calibration and characterisation includes the measurements needed to assess uncertainties at component level and their impact on the final product. 6) Post-launch calibration & characterisation covers all reasonable aspects of instrument behaviour to a quality that is "fit for purpose" in terms of the mission's stated performance. 7) All additional processing steps fully documented and state-of-the-art.	1) Persistent identifier created for all accessible data records and metadata 2) Metadata includes the identifier for the data 3) Metadata is offered in such a way that it can be harvested and indexed

USABILITY

MMP6 Data Validation

MMP7 Data Uncertainty

https://ceos.org



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ESA Earthnet Data Assessment Pilot (EDAP)

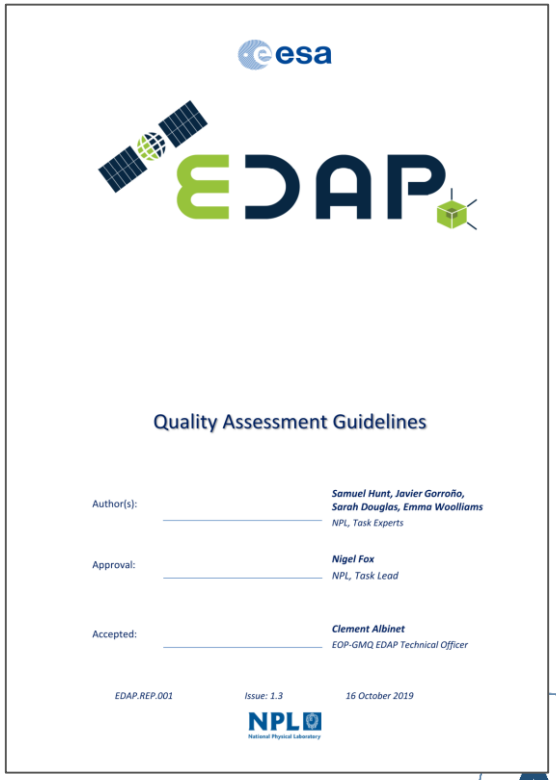
Designed for ESA and NASA assessment/endorsement of Third Party Missions

Quality Assessment Guidelines

Issue: 1.3

Product Information	Product Generation	Ancillary Information	Uncertainty Characterisation	Validation
Product Details	Sensor Calibration & Characterisation Pre-Flight	Product Flags	Uncertainty Characterisation Method	Reference Data Representativeness
Availability & Accessibility	Sensor Calibration & Characterisation Post-Launch	Ancillary Data	Uncertainty Sources Included	Reference Data Quality
Product Format	Retrieval Algorithm Method	If target mission data product is Level 2	Uncertainty Values Provided	Validation Method
User Documentation	Retrieval Algorithm Tuning		Geolocation Uncertainty	Validation Results
Metrological Traceability Documentation	Additional Processing			

Key
Not Assessed
Not Assessable
Basic
Intermediate
Good
Excellent
Information Not Public



https://earth.esa.int/eogateway/activities/edap/edap-best-practice-guidelines

SMMs in permanent evolution:
Above v1.3 (2019); currently there is v2.2 (2022), but without template or examples

Data Uncertainty

EDAP v1.3

WGISS DMSMM

	USABILITY: MMP7 DATA UNCERTAINTY		
MATURITY	**1) UNCERTAINTY METHOD**	**2) UNCERTAINTY SOURCES**	**3) UNCERTAINTY VALUES**
Level-0. Not managed	Uncertainty characterisation not performed, or method not documented	Uncertainty characterisation not performed, or sources analysed not documented.	No uncertainty information provided
Level-1. Partially managed	Limited use of GUM approach, and/or, an expanded comparison to measurements by other sensors	Most important sources of uncertainty included.	Single uncertainty value provided for subsets of data
Level-2. Managed	GUM approach to estimate measurement uncertainty with full breakdown of components and separated as Type A or B classification	All important sources of uncertainty included.	Total uncertainty per pixel is provided, with basic breakdown of key components no error covariance.
Level-3. Fully Managed.	GUM approach to estimate measurement uncertainty, including a treatment of error-covariance.	All reasonable sources of uncertainty included.	Uncertainties per pixel provided with error-covariance information for all appropriate components.

Regarding uncertainty:
EDAP v1.3 ~ WGISS + Geolocation uncertainty

Table 3-13 – Uncertainty Characterisation > Uncertainty Characterisation Method – Assessment Criteria

Grade	Criteria
Not Assessed	Assessment outside the scope of study.
Not Assessable	Uncertainty characterisation not performed, or method not documented.
Basic	Uncertainty established by limited comparison to measurements by other sensor/s Not by independent assessment and then comparison.
Intermediate	Limited use of GUM approach, and/or, an expanded comparison to measurements by other sensors.
Good	GUM approach to estimate measurement uncertainty with full breakdown of components and separated as Type A or B classification.
Excellent	GUM approach to estimate measurement uncertainty, including a treatment of error-covariance.

Table 3-14 – Uncertainty Characterisation > Uncertainty Sources Included – Assessment Criteria

Grade	Criteria
Not Assessed	Assessment outside the scope of study.
Not Assessable	Uncertainty characterisation not performed, or sources analysed not documented.
Basic	Some important sources of uncertainty missing.
Intermediate	Most important sources of uncertainty included.
Good	All important sources of uncertainty included.
Excellent	All reasonable sources of uncertainty included.

Table 3-15 – Uncertainty Characterisation > Uncertainty Values Provided – Assessment Criteria

Grade	Criteria
Not Assessed	Assessment outside the scope of study.
Not Assessable	No uncertainty information provided.
Basic	Single uncertainty value provided for whole mission.
Intermediate	Single uncertainty value provided for subsets of data, e.g. per product.
Good	Total uncertainty per pixel is provided, with basic breakdown of key components no error-covariance.
Excellent	Uncertainties per pixel provided with error-covariance information for all appropriate components.

Table 3-16 – Uncertainty Characterisation > Geolocation Uncertainty – Assessment Criteria

Grade	Criteria
Not Assessed	Assessment outside the scope of study.
Not Assessable	No uncertainty information provided
Basic	Single uncertainty value provided for whole mission.
Intermediate	Uncertainty value provided includes dependency on several variables.
Good	Uncertainty value provided includes dependency on several variables. Includes error-covariance information between pixels
Excellent	Uncertainty value provided includes dependency on several variables. Includes error-covariance information between pixels and impact on measurement uncertainty.

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Metrological Traceability

EDAP v1.3

Table 3-5 – Product Information > Metrological Traceability Documentation – Assessment Criteria

Grade	Criteria
Not Assessed	Assessment outside the scope of study.
Not Assessable	No traceability chain documented.
Basic	Traceability chain diagram and/or uncertainty tree diagram included, missing some important steps.
Intermediate	Traceability chain and/or uncertainty tree diagram documented identifying most important steps and sources of uncertainty.
Good	Rigorous uncertainty tree diagram, with, where appropriate a traceability chain documented, identifying all reasonable steps of and accompanying sources of uncertainty.
Excellent	Rigorous uncertainty tree diagram and traceability chain documented, identifying all reasonable steps and accompanying sources of uncertainty. Establishes traceability to SI.

Data Validation

EDAP v1.3

WGISS DMSMM

MATURITY GRADE	USABILITY: MMP6 DATA VALIDATION
1) Reference Data Representativeness	
Level 0	No validation activity performed.
Level 1	Reference measurements assessed to be mostly representative of the satellite measurements, covering a primary range satellite of measurements and at ad-hoc opportunities (no formal documented regular timescale).
Level 2	Reference measurements assessed to be well representative of the satellite measurements, covering a reasonable range of the satellite's measurements and carried out using FRM or community approved methods. Carried out on a regular timescale of approximately annual basis but not necessarily based on need.
Level 3	Reference measurements independently assessed to be fully representative of the satellite measurements, covering the satellite's full range of measurements and with full assessment of uncertainties and carried out on a regular basis determined by product performance.
2) Reference Data Quality	
Level 0	No validation activity performed.
Level 1	Reference data comes a single uncertainty for the entire dataset.
Level 2	Reference data comes with full uncertainty information, assessed following the GUM and traceable to community reference or SI (e.g. FRM)
Level 3	Reference data comes with full uncertainty and error-correlation information, assessed following the GUM and traceable to SI (e.g. FRM).
3) Validation Method	
Level 0	No validation activity performed.
Level 1	Methodology assess satellite measurements, simple uncertainty estimated (e.g. from statistical spread for results).
Level 2	Methodology assesses satellite measurements and reference data w.r.t. their uncertainties
Level 3	Methodology assess satellite measurements and reference data w.r.t. their error- covariance and validates those uncertainties.
4) Validation Results	
Level 0	No validation activity performed.
Level 1	Validation results show good agreement between satellite and reference measurements within uncertainties in most cases.
Level 2	Validation results show excellent agreement between satellite and reference measurements, within uncertainties. Analysis performed independently of satellite mission owner.
Level 3	Validation results show excellent agreement between satellite and reference measurements, within uncertainties. Uncertainty validated. Analysis performed independently of satellite mission owner.

Table 3-17 – Validation > Reference Data Representativeness – Assessment Criteria

Grade	Criteria
Not Assessed	Assessment outside the scope of study.
Not Assessable	No validation activity performed.
Basic	Reference measurements assessed to be somewhat representative of the satellite measurements, covering a limited range of satellite measurements. Typically, a one-off campaign.
Intermediate	Reference measurements assessed to be mostly representative of the satellite measurements, covering a primary range satellite of measurements and at ad hoc opportunities (no formal documented regular timescale).
Good	Reference measurements assessed to be well representative of the satellite measurements, covering a reasonable range of the satellite's measurements and carried out using FRM or community approved methods. Carried out on a regular timescale of approximately annual basis but not necessarily based on need.
Excellent	Reference measurements independently assessed to be fully representative of the satellite measurements, covering the satellite's full range of measurements and with full assessment of uncertainties and carried out on a regular basis determined by product performance.

Table 3-18 – Validation > Reference Data Quality – Assessment Criteria

Grade	Criteria
Not Assessed	Assessment outside the scope of study.
Not Assessable	No validation activity performed.
Basic	Uncertainty information not available for reference data.
Intermediate	Reference data comes a single uncertainty for the entire dataset.
Good	Reference data comes with full uncertainty information, assessed following the GUM and traceable to community reference or SI (e.g. FRM)
Excellent	Reference data comes with full uncertainty and error-correlation information, assessed following the GUM and traceable to SI (e.g. FRM).

Table 3-19 – Validation > Reference Data Representativeness – Assessment Criteria

Grade	Criteria
Not Assessed	Assessment outside the scope of study.
Not Assessable	No validation activity performed.
Basic	Methodology is simple comparison, uncertainties not considered.
Intermediate	Methodology assess satellite measurements, simple uncertainty estimated e.g. from statistical spread for results.
Good	Methodology assesses satellite measurements and reference data w.r.t. their uncertainties.
Excellent	Methodology assess satellite measurements and reference data w.r.t. their error-covariance and validates those uncertainties.

Table 3-20 – Validation > Validation Results – Assessment Criteria

Grade	Criteria
Not Assessed	Assessment outside the scope of study.
Not Assessable	No validation activity performed.
Basic	Validation results show some agreement between satellite and reference measurement.
Intermediate	Validation results show good agreement between satellite and reference measurements within uncertainties in most cases.
Good	Validation results show excellent agreement between satellite and reference measurements, within uncertainties. Analysis performed independently of satellite mission owner.
Excellent	Validation results show excellent agreement between satellite and reference measurements, within uncertainties. Uncertainty validated. Analysis performed independently of satellite mission owner.

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Test case: EDAP application to Sentinel-5p TROPOMI NO_2

EDAP v1.3

Product Information	Product Generation	Ancillary Information	Uncertainty Characterisation	Validation
Product Details	Sensor Calibration & Characterisation Pre-Flight	Product Flags	Uncertainty Characterisation Method	Reference Data Representativeness
Availability & Accessibility	Sensor Calibration & Characterisation Post-Launch	Ancillary Data	Uncertainty Sources Included	Reference Data Quality
Product Format	Retrieval Algorithm Method		Uncertainty Values Provided	Validation Method
User Documentation	Retrieval Algorithm Tuning		Geolocation Uncertainty	Validation Results
Metrological Traceability Documentation	Additional Processing			

Key
Not Assessed
Not Assessable
Basic
Intermediate
Good
Excellent
Information Not Public

Work in progress…

Product Details	
Product Name	*Sentinel-5P\TROPOMI Level 2 Nitrogen dioxide [L2__NO2___]*
Sensor Name	*TROPOMI*
Sensor Type	*nadir-viewing, imaging spectrometer covering wavelength bands between the ultraviolet and the shortwave infrared*
Mission Type	*Single satellite mission. But in loose constellation with Suomi-NPP\VIIRS.*
Mission Orbit	*Low Earth orbit near-polar sun-synchronous, ascending node equatorial crossing at 13:30 h local solar time*
Product Version Number	*1.2.0, 1.2.2, 1.3.0, 1.3.1, 1.3.2, 1.4.0, 2.2.0, 2.3.1*
Product ID	*L2__NO2___. File class denoting timeliness: RPRO, OFFL, NRTI*
Processing level of product	*Level 2*
Measured Quantity Name	*Stratospheric NO2 vertical column density* *Tropospheric NO2 vertical column density* *Total NO2 vertical column density*
Measured Quantity Units	*mol m-2*
Stated Measurement Quality	*Concluded by validation: In overall agreement with reference data (ground-based+OMI)and compliant with requirements [PRF-NO2]*
Spatial Resolution	*3.5 x 7.0 Km (across x along track), at beginning of mission* *3.5 x 5.5 Km (across x along track), since 6 August 2019*
Spatial Coverage	*~2600 km swath. Full daily surface coverage of radiance and reflectance measurements for latitudes > 7° and < -7°, and better than 95 % coverage for latitudes in the interval [-7°, 7°].*
Temporal Resolution	*Revisit time: 1 day or less*
Temporal Coverage	V2: Since 01-Jul-2021 V1: Since 30-Apr-2018 to 01-Jul-2021
Point of Contact	European Space Agency, EOSupport@Copernicus.esa.int
Product locator (DOI/URL)	V2, OFFL: https://doi.org/10.5270/S5P-9bnp8q8 V1, OFFL: https://doi.org/10.5270/S5P-s4ljg54
Conditions for access and use	Free, full and open access to Copernicus Sentinel Data 2 and Service Information without any express or implied warranty See https://sentinels.copernicus.eu/documents/247904/690755/Sentinel_Data_Legal_Notice
Limitations on public access	Accessible via doi
Product Abstract	Short abstract available via https://sentinels.copernicus.eu/web/sentinel/data-products/

tinel-5p TROPOMI NO_2

Product details

Table 3-1 – Product Information > Product Details – Assessment Criteria

Grade	Criteria
Not Assessed	Assessment outside of the scope of study.
Not Assessable	Relevant information not made available.
Basic	Some pieces of required information missing.
Intermediate	Any required information missing.
Good	All required information available, any recommended information missing.
Excellent	All required and recommended information available.

Conclusion:
Good to Excellent – Almost all required and recommended information available

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Test case: EDAP application to Sentinel-5p TROPOMI NO_2

Product Format	
Product File Format	*netCDF-4*
Metadata Conventions	[PUM-NO2]: Metadata items are included following conventions • In group METADATA, to facilitate dataset discovery: Earth Observation – Ground segment file format standard [RD35], INSPIRE [ER4], ISO 19115 [RD36], ISO 19115-2 [RD37], ISO 19157 [RD38] and OGC 10-157r3 [RD39]. • Global attributes: Climate and Forecast (CF) metadata conventions [ER5], the Attribute Convention for Dataset Discovery [ER6], the NetCDF-4 user guide (NUG) [ER7] and the ESA CCI project [RD40] • Variable attributes from CF and NUG conventions are included.
Analysis Ready Data?	*Not assessed*

Product format

Table 3-3 – Product Information > Product Format – Assessment Criteria

Grade	Criteria
Not Assessed	Assessment outside the scope of study.
Not Assessable	Non-standard, undocumented data format.
Basic	Non-standard or proprietary data format, or, poorly-documented standard file format.
Intermediate	Data in documented standard file format. Non-standard naming conventions used.
Good	Data in well-documented standard file format, meeting community naming convention standards.
Excellent	Analysis Ready Data standard if applicable, else as *Good*.

Conclusion.

Good to Excellent. Data are organized a well-documented standard file format, meeting community naming convention standards. Comprehensive set of metadata and data flags.

Analysis Ready Data: certification procedures not yet developed for Atmospheric missions

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Test case: EDAP application to Sentinel-5p TROPOMI NO_2

User Documentation		
Document	*Reference*	*QA4ECV Compliant*
Product User Guide	*1/ S5P Mission Performance Centre Nitrogen Dioxide [L2__NO2__] Readme [PRF-NO2] 2/ Sentinel-5 precursor/TROPOMI Level 2 Product User Manual Nitrogendioxide [PUM-NO2]*	*Yes, for the most part. Missing: (1) How to use the uncertainty data. (2) Case studies.*
ATBD	*TROPOMI ATBD of the total and tropospheric NO2 data products [ATBD-NO2]*	*Yes, for the most part. Missing: (1) parameter definition in introduction. (2) list of assumptions*

User Documentation

Table 3-4 – Product Information > User Documentation – Assessment Criteria

Grade	Criteria
Not Assessed	Assessment outside the scope of study.
Not Assessable	No user documentation provided, or, documentation out-of-date.
Basic	Limited PUG available, no ATBD. Documentation up-to-date.
Intermediate	Some PUG and ATBD-type information available. May be as formal documents or made up of e.g. articles. Documentation up-to-date.
Good	PUG meeting QA4ECV standard, reasonable ATBD. Documentation up-to-date.
Excellent	PUG ATBD available meeting QA4ECV standard. Documentation up-to-date.

Conclusion.

Good to Excellent. Almost QA4ECV compliant and up to date.

Test case: CEOS DMSMM Application to candidate FRM data

WGISS Data Uncertainty maturity criteria applied to
Ground-based Direct-sun DOAS Pandora data (v1.8) from Pandonia Global Network.

UNCERTAINTY ASPECT	MATURITY LEVEL (0 TO 3)
Uncertainty Method	Level 3. GUM approach to estimate measurement uncertainty, including a treatment of error covariance.
Uncertainty Sources	Level 3. All important* sources of uncertainty included.
Uncertainty Values	Level 3. Total uncertainty per pixel provided with error covariance information for all appropriate components

*Note that no formal error covariance matrix is provided, but uncertainty is distinguished between common (fully correlated in time), independent (not correlated) and structured (intermediately correlated).

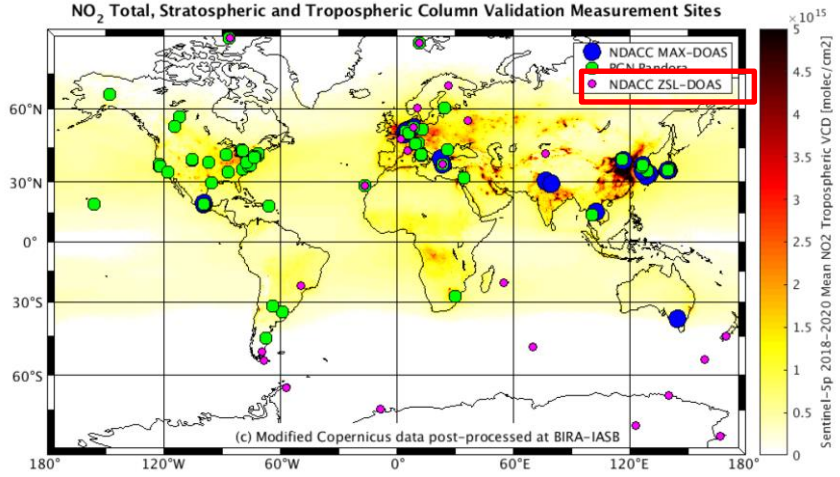
Source: Precursors_cci+ Product Validation Plan 2023, S. Compernolle and J.-C. Lambert

https://climate.esa.int/en/projects/precursors-for-aerosols-and-ozone/

Source: Precursors_cci+ Product Validation Plan 2023, S. Compernolle and J.-C. Lambert

Test case: Maturity of Validation Data

Precursors_cci+ stratospheric NO2 VCD Climate Data Record (1995-now) vs NDACC ZSL-DOAS (80'-now)

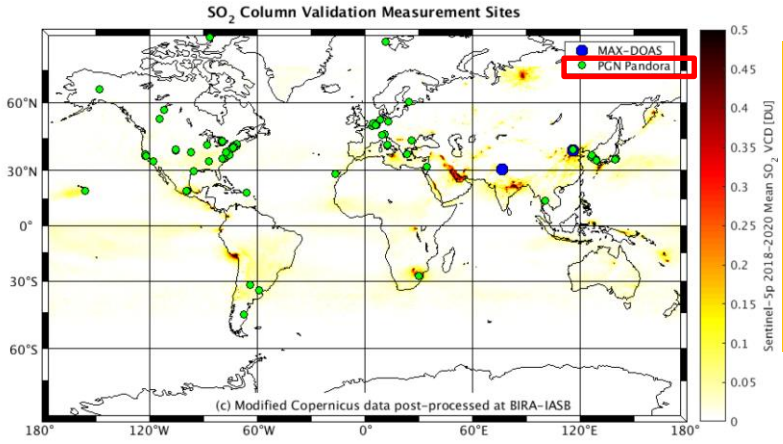


Good geographical & temporal coverage
→ *Good (level 2) Data Representativeness*

Table 12. WGISS Data Validation maturity applied to the validation of stratospheric NO2 VCD using ZSL-DOAS.

DATA VALIDATION ASPECT	MATURITY
Reference Data Representativeness	Level-2. Reference measurements assessed to be well representative of the satellite measurements, covering a reasonable range of the satellite's measurements and carried out using FRM or community approved methods. Carried out on a regular timescale of approximately annual basis but not necessarily based on need.
Reference Data Quality	Level 2. Reference data comes with full uncertainty information, assessed following the GUM and traceable to community reference or SI (e.g. FRM)
Validation Method	Level 3. Methodology assess satellite measurements and reference data w.r.t. their error- covariance and validates those uncertainties.
Validation Results	*Will be assessed in PVIR*

Precursors_cci+ tropo SO2 VCD Climate Data Record (1995-now) vs PGN Pandora (2018-now)



Wide geographical coverage but recent data only and lack of polluted sites
→ *Poor (level 0-1) Data Representativeness*

Table 13. WGISS Data validation maturity applied to the validation of tropospheric SO2 VCD using PGN Pandora.

DATA VALIDATION ASPECT	MATURITY
Reference Data Representativeness	Between Level-0 No validation activity performed and Level 1: Reference measurements assessed to be mostly representative of the satellite measurements, covering a primary range satellite of measurements and at ad-hoc opportunities (no formal documented regular timescale).
Reference Data Quality	Level 2. Reference data comes with full uncertainty information, assessed following the GUM and traceable to community reference or SI (e.g. FRM)
Validation Method	Level 2. Methodology assesses satellite measurements and reference data w.r.t. their uncertainties
Validation Results	*Will be assessed in PVIR*

Mapping TUNER recommendations and EDAP System Maturity Matrix (preliminary)

TUNER framework paper		EDAP v1.3
R 1. The language and notation used to describe the error budget must be clearly defined.	⟷	'**Uncertainty Methods**': Good (*GUM methodology implies GUM/VIM terminology*)
R 2. Error budget as complete as possible, i.e., all size-able sources included	⟷	'**Uncertainty Sources**': Good to Excellent
R 3. Report substantive contributions from each relevant error component separately	⟷	'**Uncertainty Methods+Values**': Good to Excellent
R 4. Report per error source dependencies between data subsets in a certain domain (time, space, species, etc.).	⟷	'**Uncertainty Values**': Excellent *(error correlation between pixels for all relevant components)*
R 5. Report per error component: contributing to random/volatile or systematic/persistent error ?	⟷	*Not separately treated from above (error correlation)*
R 6. Clarify meaning of reported uncertainties (e.g., 1-sigma, 95% confidence)	⟷	'**Uncertainty Methods**': Good *(Implied by GUM methodology)*

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Mapping TUNER recommendations and EDAP System Maturity Matrix (preliminary)

TUNER framework paper		EDAP v1.3
R 7. Report for all error components, ingoing uncertainties+correlation in documentation.	⟺	'**Metrological traceability documentation**': Good to Excellent. *No focus on correlation.*
R 8 to R 12 are about a priori and AK	⟺	*Not explicitly covered.* *Could have its place in* '**Ancillary Data**'
R 13 to R 17 about representative cases to limit data volume	⟺	This would limit grading in '**Uncertainty values**' to Intermediate.
R 18. The error estimates should explain observed differences between measurements of the same air mass. • Random/volatile • Systematic/persistent	⟺	*Random/systematic split not explicitly covered.* Could have its place in '**Validation Results**'

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Conclusions and outlook

- EDAP and WGISS System Maturity Matrices are being applied to satellite data products.
- Tentatively, they are being adapted and applied to ground-based data as candidate FRMs.
- TUNER recommendations could contribute to more detailed maturity criteria.

- EDAP v1.3 to v2.2: impact of the change on the maturity assessments?

Mission Quality Assessment Guidelines v1.3

1.1 Mission Quality Assessment Matrix

Product Information	Product Generation	Ancillary Information	Uncertainty Characterisation	Validation
Product Details	Sensor Calibration & Characterisation Pre-Flight	Product Flags	Uncertainty Characterisation Method	Reference Data Representativeness
Availability & Accessibility	Sensor Calibration & Characterisation Post-Launch	Ancillary Data	Uncertainty Sources Included	Reference Data Quality
Product Format	Retrieval Algorithm Method	If target mission data product is Level 2	Uncertainty Values Provided	Validation Method
User Documentation	Retrieval Algorithm Tuning		Geolocation Uncertainty	Validation Results
Metrological Traceability Documentation	Additional Processing			

Key
Not Assessed
Not Assessable
Basic
Intermediate
Good
Excellent

Information Not Public

Mission Quality Assessment Guidelines v2.2

Data Provider Documentation Review			Validation Summary
Product Information	Metrology	Product Generation	
Product Details	Radiometric Calibration & Characterisation	Radiometric Calibration Algorithm	Radiometric Validation Method
Availability & Accessibility	Geometric Calibration & Characterisation	Geometric Processing	Radiometric Validation Results Compliance
Product Format, Flags & Metadata	Metrological Traceability Documentation	Retrieval Algorithm	Geometric Validation Method
User Documentation	Uncertainty Characterisation	Mission-Specific Processing	Geometric Validation Results Compliance
	Ancillary Data		

Key
Not Assessed
Not Assessable
Basic
Good
Excellent
Ideal
Not Public