# Precursors_cci+

# ESA Climate Change Initiative (CCI)



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## Table of Contents

EXECUTIVE SUMMARY 7

1. INTRODUCTION 9

1.1. Purpose and scope 9

1.2. Document overview 10

2. APPLICABLE AND REFERENCE DOCUMENTS 11

2.1. Applicable documents 11

2.2. Reference documents 11
2.2.1. Project documents 11
2.2.2. Climate data user requirement documents 11
2.2.3. Standards and framework documents 11
2.2.4. Ground-based (reference) measurements 12
2.2.4.1. Zenith-scattered-light UV-Visible DOAS (ZSL-DOAS) 12
2.2.4.2. Pandora / Pandonia Global Network (PGN) 13
2.2.4.3. Multi-axis UV-Visible DOAS (MAX-DOAS) 13
2.2.4.4. Fourier Transform Infra-Red spectrometry (FTIR) 15
2.2.4.5. Cloud monitoring network (Cloudnet) 15
2.2.5. Geophysical validation 15
2.2.5.1. Level-2 data validation protocol 15
2.2.5.2. Level-3 data validation protocol 16
2.2.5.3. $NO_2$ column validation 16
2.2.5.4. HCHO column validation 17
2.2.5.5. $SO_2$ column validation 18
2.2.5.6. CO column validation 18
2.2.5.7. $NH_3$ column validation 18
2.2.5.8. CHOCHO column validation 19
2.2.5.9. Cloud height validation 19
2.2.5.10. Geostationary product validation 19
2.2.5.11. Methods, models, tools and miscellaneous 20

3. USER REQUIREMENTS 22

3.1. URD requirements from user survey 22

3.2. Numerical quality requirements in 2022 GCOS IP and in URD 23
3.2.1. Generalities 23
3.2.2. Tropospheric nitrogen dioxide column 24
3.2.3. Tropospheric formaldehyde column 24
3.2.4. Tropospheric sulphur dioxide column 24
3.2.5. Tropospheric carbon monoxide column 26
3.2.6. Tropospheric ammonia column 26
3.2.7. Tropospheric glyoxal column 26

3.3. Data format and metadata conventions 28

4. ECV DATA PRODUCT VALIDATION PROTOCOL 29

4.1. Generic principles applicable to all ECVs 29
4.1.1. Validation protocol for atmospheric composition satellites 29
4.1.2. Maturity assessment of satellite data validation 32
4.1.3. Validation against user requirements 33
4.1.4. Validation metrics and their link with user requirements 34
4.1.5. Tools and auxiliary data 35
4.1.6. Validation of individual processing components 35
4.1.7. Error budget closure of a data comparison 36
4.1.8. Satellite data intercomparison 37
4.1.9. Level-3 data validation 38

4.2. Validation specifics by ECV 40
4.2.1. Quantities with potential impact on ECV data quality 40
4.2.2. Validation requirements common to all data products 40
4.2.3. Tropospheric $NO_2$ data product 41
4.2.3.1. Validation requirements 41
4.2.3.2. Validation data sources 41
4.2.3.3. Maturity of Data Validation 41
4.2.4. Tropospheric HCHO data product 42
4.2.4.1. Validation requirements 42
4.2.4.2. Validation data sources 42
4.2.5. Tropospheric $SO_2$ data product 43
4.2.5.1. Validation requirements 43
4.2.5.2. Validation data sources 43
4.2.5.3. Maturity of Data Validation 43
4.2.6. Tropospheric CO data product 44
4.2.6.1. Validation requirements 44
4.2.6.2. Validation data sources 44
4.2.7. $NH_3$ data product 44
4.2.7.1. Validation requirements 44
4.2.7.2. Validation data sources 44
4.2.8. CHOCHO data product 44
4.2.8.1. Validation requirements 44
4.2.8.2. Validation data sources 45
4.2.9. Validation approach to data from geostationary missions 45
4.2.9.1. Validation needs 45
4.2.9.2. Recommendation on time range to be processed 45
4.2.9.3. Planned work 46

5. REFERENCE MEASUREMENTS 48

5.1. Maturity of reference measurements 49
5.1.1. Maturity as a Fiducial Reference Measurement 49
5.1.2. Maturity of associated uncertainty estimates 50

5.2. Data access and policy of ground-based monitoring networks 51
5.2.1. The Network for the Detection of Atmospheric Composition Change (NDACC) 51
5.2.2. The Pandonia Global Network (PGN) 52
5.2.3. The Total Carbon Column Observing Network (TCCON) 53

5.2.4. The Cloudnet network in the ACTRIS Research Infrastructure 55

5.3. NDACC Zenith-Scattered-Light (ZSL-) UV-visible DOAS data 57
5.3.1. Description 57
5.3.2. Geographical and temporal coverage and sampling 57
5.3.3. Data access and data access policy 59
5.3.4. Uncertainty characteristics 59
5.3.5. Limitations 59

5.4. Multi-Axis (MAX-) UV-visible DOAS data 60
5.4.1. Description 60
5.4.2. Geographical and temporal coverage and sampling 60
5.4.2.1. MAX-DOAS $NO_2$ measurements 60
5.4.2.2. MAX-DOAS HCHO measurements 61
5.4.2.3. MAX-DOAS SO2 measurements 63
5.4.2.4. MAX-DOAS CHOCHO measurements 63
5.4.3. Data access and data access policy 64
5.4.4. Uncertainty characteristics 65
5.4.5. Limitations 65

5.5. Direct-Sun UV-visible DOAS data 66
5.5.1. Description 66
5.5.2. Geographical and temporal coverage and sampling 66
5.5.2.1. Direct-sun DOAS $NO_2$ measurements 66
5.5.2.2. Direct-sun DOAS $SO_2$ measurements 68
5.5.3. Data access and data access policy 70
5.5.4. Uncertainty characteristics 70
5.5.5. Limitations 70
5.5.6. Maturity as a Fiducial Reference Measurement 71
5.5.7. Maturity of Data Uncertainty estimates 71

5.6. Fourier Transform Infra-Red spectrometer data 72
5.6.1. Description 72
5.6.2. Geographical and temporal coverage and sampling 72
5.6.2.1. FTIR HCHO measurements 72
5.6.2.2. FTIR CO measurements 73
5.6.2.3. FTIR $NH_3$ measurements 75
5.6.3. Data access and data access policy 77
5.6.4. Uncertainty characteristics 77
5.6.5. Limitations 78

5.7. Cloudnet radar/lidar data 79
5.7.1. Description 79
5.7.2. Data access and data access policy 79
5.7.3. Geographical and temporal coverage and sampling 79
5.7.4. Uncertainty characteristics 80
5.7.5. Limitations 80

6. COMPLIANCE WITH DOCUMENT REQUIREMENT DEFINITIONS 81

7. TERMS, ABBREVIATIONS AND DEFINITIONS 82

7.1. Terms and definitions 82

7.2. Abbreviations and acronyms 85

7.3. Validation metadata 87

# Executive Summary

This document is the *Product Validation Plan* (PVP) Version 03 of the ESA CCI+ Precursors project (hereafter Precursors_cci+). The PVP defines the approach to the geophysical validation of the satellite-based Essential Climate Variables (ECV) data produced by the project that shall be applied in the Product Validation and Intercomparison Report (PVIR). The PVP Version 03 represents the status of the validation plan in cycle 2 of the Precursors_cci+ project and is not intended to be a public document.

The ozone and aerosols ECV precursors data products produced by the project are:

Based on observations from the UV-visible nadir sounders GOME, SCIAMACHY, GOME-2A, -2B and -2C, OMI and TROPOMI:
(i) nitrogen dioxide ($NO_2$) tropospheric column,
(ii) formaldehyde (HCHO) tropospheric column,
(iii) sulphur dioxide ($SO_2$) total column.

Based on observations from infrared nadir sounders:
(iv) carbon monoxide (CO) column (observations from MOPITT and IASI-A, -B and -C),
(v) ammonia ($NH_3$) column (observations from IASI-A, -B and -C).

Based on observations from GOME-2A, -2B and -2C, OMI and TROPOMI:
(vi) glyoxal (CHOCHO) column.

User requirements outlined in *The 2022 GCOS Implementation Plan* and the Precursors_cci+ *User Requirements Document* (URD) are translated into validation requirements. The adopted validation protocol, validation standards, validation metrics and validation tools are described. The maturity and limitations of the validation methods are evaluated.

Validation of the satellite-based Climate Data Records relies substantially on comparisons against independent ground-based measurements of known quality used as a reference, complemented by *ad hoc* cross-validation with other satellite-based datasets. The ground-based measurements considered as a reference in this validation plan (hereafter Fiducial Reference Measurements, FRM) are collected from: (i) NDACC zenith-scattered-light DOAS spectrometers (ZSL-DOAS) for the validation of stratospheric NO2 column data, (ii) multi-axis DOAS instruments (MAX-DOAS) for the validation of tropospheric $NO_2$, HCHO, $SO_2$ and CHOCHO columns, (iii) PGN/Pandora direct-Sun DOAS instruments for the validation of $NO_2$ and $SO_2$ columns, (iv) NDACC FTIR direct-Sun spectrometers for the validation of HCHO, CO and $NH_3$ columns, and (v) TCCON FTIR direct-Sun spectrometers for the validation of CO columns.

For each ECV precursor the FRM datasets are described, including a first assessment of their uncertainty characteristics, limitations, availability, access, and data policy. Initial (illustrative) assessments of the maturity of the FRMs for validation purposes are provided. Compared to previous PVP versions, this PVP Version 03 provides a more detailed analysis of the FRM datasets, including a consolidated evaluation of the geographical and temporal coverage and

sampling currently available to the project. It also includes now the validation approach to geostationary missions, while previous versions were limited to low-Earth orbiting missions.

# 1. Introduction

## 1.1. Purpose and scope

This *Product Validation Plan* (PVP) describes the validation requirements and validation plans for the Climate Data Records (CDR) of ozone and aerosol Essential Climate Variable (ECV) Precursors to be generated by the ESA Precursors_cci+ project, namely:

Based on observations from the UV-visible nadir sounders ERS-2 GOME, Envisat SCIAMACHY, MetOp GOME-2A, -B and -C, EOS-Aura OMI, and Sentinel-5P TROPOMI:

(vii) nitrogen dioxide ($NO_2$) tropospheric column,
(viii) formaldehyde (HCHO) column,
(ix) sulphur dioxide ($SO_2$) column.

Based on observations from infrared nadir sounders:

(x) carbon monoxide (CO) column (observations from EOS-Terra MOPITT and MetOp IASI-A, -B and -C),
(xi) ammonia ($NH_3$) column (observations from MetOp IASI-A, -B and -C).

Based on observations from MetOp GOME-2A, -2B and -2C, EOS-Aura OMI, and Sentinel-5P TROPOMI:

(xii) glyoxal (CHOCHO) column.

The objective of the planned validation activities is to associate to each CDR produced by the project a set of fully traceable Quality Indicators (QI) enabling users to readily assess the fitness for purpose of the data. Quality Indicators shall be defined such that they enable verification of compliance of the data products with user requirements expressed in the Precursors_cci+ *User Requirements Document* (URD). The latter includes requirements for the Global Climate Observing System (GCOS) as well as requirements collected from the climate research and remote sensing communities. The PVP on ECV precursors is grounded on the heritage of past and current validation activities including those performed in the framework of the EC FP7 project Quality Assurance for ECV (QA4ECV), the ESA Ozone_cci and GHG_cci projects, the ESA/Copernicus Sentinel-5p Atmospheric Mission Performance Cluster (ATM-MPC), and the EUMETSAT Satellite Application Facility on Atmospheric Composition (AC SAF). The present PVP update to version 03 includes plans for the validation of ECV datasets acquired by geostationary satellite missions, as pioneered in ESA's project PEGASOS and NIER/Yonsei's project Geo-Ring.

This Version 3 of the *Product Validation Plan* represents the status at cycle 3 of the Precursors_cci+ project. The validation protocol, expected outcome, and planned Quality Indicators are described in detail. Special care has been given to the discovery and characterization of the ground-based measurements to be used as a reference for ECV CDR validation, and to the evaluation of their maturity as a Fiducial Reference Measurement (FRM). This version 3 takes into account the outcome of and lessons learnt from the first two cycles, Version 1 of the *Product Validation and Algorithm Selection Report* (PVASR) [RD6:PVASR] and Version 2 of the *Product Validation and Intercomparison Report* (PVIR) [RD8:PVIRv2].

## 1.2. Document overview

This *Product Validation Plan* Version 1 is structured as follows:

- **Section 1** contains this introduction describing the purpose and scope of the document.
- **Section 2** lists applicable and reference documents.
- **Section 3** reproduces the relevant user requirements against which Climate Data Records of ECV precursors shall be validated.
- **Section 4** defines the validation protocol for the final ECV data products. It starts with generic principles of atmospheric data validation, and it details the specifics with regard to the validation of the six different ECV precursors.
- **Section 5** describes the characteristics of the ground-based measurements planned to be used as a reference, and proposes a FRM Maturity Assessment Procedure (FRM-MAP) applicable to every source.
- **Section 6** maps the content of this document with the Document Requirement Definitions outlined in Annex A of the Precursors_cci+ Statement of Work.
- **Section 7** defines the recommended terminology, abbreviations and acronyms; it also defines the metadata to associate with every set of validation results.

# 2. Applicable and reference documents

## 2.1. Applicable documents

[RD1:BP] Precursors CCI+ Baseline proposal. CCI+ Phase 2 – New ECVs: Precursors for Aerosol and Ozone ECV, Proposal to ESA in response to ITT AO/1-11036/21/I-NB. Technical Baseline Proposal.

[RD2:OP] Precursors CCI+ Optional proposal. CCI+ Phase 2 – New ECVs: Precursors for Aerosol and Ozone ECV. Proposal to ESA in response to ITT AO/1-11036/21/I-NB. Optional Proposal.

[RD3:EP] Extension of Precursors_CCI+ activities. Detailed proposal to ESA. CCN-01 to contract No. 4000138243/22/I-NB, 2025/04/09.

[RD4:DRD] CCI+ Phase 2 Theme (I) - Precursors ECV SoW - Annex A – Document Requirement Definitions, Issue 1.2, ESA-EOP-SC-SP-2021-38, 06/08/2021.

## 2.2. Reference documents

### 2.2.1. Project documents

[RD5:PVPv2] Precursors CCI+ Product Validation Plan (PVP), deliverable 1.3, issue 2, revision 1, Precursors_cci+_D1.3_PVP_01_01, 5 Aug 2024.

[RD6:PVASR] Precursors CCI+ Product Validation and Algorithm Selection Report (PVASR), deliverable 2.3, issue 1, Precursors_cci+_D2.3_PVASR_01_00, 29 Feb 2024.

[RD7:PUG] Precursors CCI+ Product User Guide, deliverable 4.2, Precursors_cci+_D4.2_PUG_01_01.

[RD8:PVIRv2] Precursors CCI+ Product Validation and Intercomparison Report, deliverable 4.1, issue 2, Precursors_cci+_D4.1_PVIR_02_00, 23 Sep 2025.

### 2.2.2. Climate data user requirement documents

[RD9:GCOS_IP] The 2022 GCOS Implementation Plan. GCOS-244. GOOS-272. 98 pp. © World Meteorological Organization, 2022. https://gcos.wmo.int/en/publications/gcos-implementation-plan2022

[RD10:GCOS_Req] The 2022 GCOS ECVs Requirements. GCOS-245. (Supplement to the 2022 GCOS Implementation Plan). 244 pp. © World Meteorological Organization, 2022. https://gcos.wmo.int/en/publications/gcos-implementation-plan2022

[RD11:URD] Precursors CCI+ User Requirement Document, deliverable 1.1, Precursors_cci+_D1.1_URD_00_02, draft version.

### 2.2.3. Standards and framework documents

[RD12:QA4EO] A Quality Assurance Framework for Earth Observation (QA4EO), Implementation Strategy and Work Plan, March 2012, version 0.4, http://qa4eo.org/docs/qa4eo_implementation_strategy_for_ceos_and_geo_v0_4.pdf

[RD13:CEOS] Committee on Earth Observation Satellites (CEOS): Terms and Definitions and other documents and resources, publicly available on http://calvalportal.ceos.org

[RD14:GUM] Joint Committee for Guides in Metrology (JCGM/WG 1) 100:2008, Evaluation of measurement data – Guide to the expression of uncertainty in a measurement (GUM), http://www.bipm.org/utils/common/documents/jcgm/JCGM_100_2008_E.pdf

[RD15:VIM] Joint Committee for Guides in Metrology (JCGM/WG 2) 200:2012, International vocabulary of metrology – Basic and general concepts and associated terms (VIM), www.bipm.org/utils/common/documents/jcgm/JCGM_200_2012.pdf

[RD16:FRM_def] C. Donlon and G. Zibordi, In situ optical radiometry, Chapter 3 of Optical Radiometry for Ocean Climate Measurements, Eds. G. Zibordi, C. Donlon and A. Parr, EMPS Series, Vol. 47, Elsevier Inc., ISBN: 978-0-12-417011-7, 2014

[RD17:WGIS_MM] CEOS WGISS Data Management & Stewardship Maturity Matrix. CEOS.WGISS.DSIG.DSMM. Version 1.3. 2020, https://ceos.org/document_management/Working_Groups/WGISS/Interest_Groups/Data_Stewardship/White_Papers/WGISS%20Data%20Management%20and%20Stewardship%20Maturity%20Matrix.pdf

[RD18:CF] NetCDF Climate and Forecast Metadata Convention, http://cfconventions.org

[RD19:CCI_standard] CCI Data Standards, version 2.3, CCI-PRGM-EOPS-TN-13-0009, ESA Climate Office, 26/07/2021. https://climate.esa.int/documents/1284/CCI_DataStandards_v2-3.pdf

[RD:CEOS-FRM] Goryl, P., Fox, N., Donlon, C., Castracane, P., Fiducial Reference Measurements (FRMs): What Are They? Remote Sens. 2023, 15, 5017. https://doi.org/10.3390/rs15205017

### 2.2.4. Ground-based (reference) measurements

#### 2.2.4.1. Zenith-scattered-light UV-Visible DOAS (ZSL-DOAS)

[RD20:Solomon1987] Solomon, S.; Schmeltekopf, A. L. & Sanders, R. W. On the interpretation of zenith sky absorption measurements, *J. Geophys. Res.,* **1987***, 92*, 8311-8319

[RD21:Bognar2019] Bognar, K., Zhao, X., Strong, K., Boone, C., Bourassa, A., Degenstein, D., Drummond, J., Duff, A., Goutail, F., Griffin, D., Jeffery, P., Lutsch, E., Manney, G., McElroy, C., McLinden, C., Millán, L., Pazmino, A., Sioris, C., Walker, K., and Zou, J.: Updated validation of ACE and OSIRIS ozone and NO2 measurements in the Arctic using ground-based instruments at Eureka, Canada, J. Quant. Spectrosc. Ra., 238, 106571, https://doi.org/10.1016/j.jqsrt.2019.07.014, 2019.

[RD22:Roscoe1999] Roscoe, H., Johnston, P., Van Roozendael, M., Richter, A., Sarkissian, A., Roscoe, J., Preston, K., Lambert, J.-C., Hermans, C., De Cuyper, W., Dzienus, S., Winterrath, T., Burrows, J., Goutail, F., Pommereau, J.-P., D'Almeida, E., Hottier, J., Coureul, C., Ramon, D., Pundt, I., Bartlett, L., McElroy, C., Kerr, J., Elokhov, A., Giovanelli, G., Ravegnani, F., Premuda, M., Kostadinov, I., Erle, F., Wagner, T., Pfeilsticker, K., Kenntner, M., Marquard, L., Gil, M., Puentedura, O., Yela, M., Arlander, W., Kåstad Høiskar, B., Tellefsen, C., Karlsen Tørnkvist, K., Heese, B., Jones, R., Aliwell, S., and

Freshwater, R.: Slant column measurements of O3 and NO2 during the NDSC intercomparison of zenith-sky UV-visible spectrometers in June 1996, J. Atmos. Chem., 32, 281–314, 1999.

[RD23:Hendrick2004] Hendrick, F., Barret, B., Van Roozendael, M., Boesch, H., Butz, A., De Mazière, M., Goutail, F., Hermans, C., Lambert, J.-C., Pfeilsticker, K., and Pommereau, J.-P.: Retrieval of nitrogen dioxide stratospheric profiles from ground-based zenith-sky UV-visible observations: validation of the technique through correlative comparisons, Atmos. Chem. Phys., 4, 2091–2106, https://doi.org/10.5194/acp-4-2091-2004, 2004.

[RD24:Vandaele2005] Vandaele, A. C., et al. (2005), An intercomparison campaign of ground-based UV-visible measurements of NO2 , BrO, and OClO slant columns: Methods of analysis and results for NO2, J. Geophys. Res., 110, D08305, doi:10.1029/2004JD005423.

[RD25:Yela2017] Yela, M., Gil-Ojeda, M., Navarro-Comas, M., Gonzalez-Bartolomé, D., Puentedura, O., Funke, B., Iglesias, J., Rodríguez, S., García, O., Ochoa, H., and Deferrari, G.: Hemispheric asymmetry in stratospheric NO2 trends, Atmos. Chem. Phys., 17, 13373–13389, https://doi.org/10.5194/acp-17-13373-2017, 2017.

#### 2.2.4.2. Pandora / Pandonia Global Network (PGN)

[RD26:Herman2009] Herman, J., A. Cede, E. Spinei, G. Mount, M. Tzortziou, and N. Abuhassan (2009), NO 2 column amounts from ground-based Pandora and MFDOAS spectrometers using the direct-sun DOAS technique: Intercomparisons and application to OMI validation, J. Geophys. Res., 114, D13307, doi:10.1029/2009JD011848.

[RD27:Fioletov2016] Fioletov, V. E., McLinden, C. A., Cede, A., Davies, J., Mihele, C., Netcheva, S., Li, S.-M., and O'Brien, J.: Sulfur dioxide ($SO_2$) vertical column density measurements by Pandora spectrometer over the Canadian oil sands, Atmos. Meas. Tech., 9, 2961–2976, https://doi.org/10.5194/amt-9-2961-2016, 2016.

[RD28:FRM4AQ] Fiducial Reference Measurements for Air Quality, New Algorithm & Product Development Plan, Version 7.0, 28 th June 2022, LuftBlick Report 2019005, https://www.pandonia-global-network.org/wp-content/uploads/2022/08/LuftBlick_FRM4AQ_NewAlgorithmPlan-ATBD_RP_2019005_v7.pdf

[RD29:Tiefengraber2017] Martin Tiefengraber, Luftblick, private communication to Steven Compernolle, 2022/12/07.

#### 2.2.4.3. Multi-axis UV-Visible DOAS (MAX-DOAS)

[RD30:Hönninger2004] Hönninger, G., von Friedeburg, C., and Platt, U.: Multi axis differential optical absorption spectroscopy (MAX-DOAS), Atmos. Chem. Phys., 4, 231–254, https://doi.org/10.5194/acp-4-231-2004, 2004.

[RD31:Hendrick2014] Hendrick, F., Müller, J.-F., Clémer, K., Wang, P., De Mazière, M., Fayt, C., Gielen, C., Hermans, C., Ma, J. Z., Pinardi, G., Stavrakou, T., Vlemmix, T., and Van Roozendael, M.: Four years of ground-based MAX-DOAS observations of HONO and $NO_2$ in the Beijing area, Atmos. Chem. Phys., 14, 765–781, https://doi.org/10.5194/acp-14-765-2014, 2014.

[RD32:Friedrich2019] Friedrich, M. M., Rivera, C., Stremme, W., Ojeda, Z., Arellano, J., Bezanilla, A., García-Reynoso, J. A., and Grutter, M.: $NO_2$ vertical profiles and column densities from MAX-DOAS measurements in Mexico City, Atmos. Meas. Tech., 12, 2545–2565, https://doi.org/10.5194/amt-12-2545-2019, 2019

[RD33:Bösch2018] Bösch, T., Rozanov, V., Richter, A., Peters, E., Rozanov, A., Wittrock, F., Merlaud, A., Lampel, J., Schmitt, S., de Haij, M., Berkhout, S., Henzing, B., Apituley, A., den Hoed, M., Vonk, J., Tiefengraber, M., Müller, M., and Burrows, J. P.: BOREAS – a new MAX-DOAS profile retrieval algorithm for aerosols and trace gases, Atmos. Meas. Tech., 11, 6833–6859, https://doi.org/10.5194/amt-11-6833-2018, 2018.

[RD34:Irie2011] Irie, H., Takashima, H., Kanaya, Y., Boersma, K. F., Gast, L., Wittrock, F., Brunner, D., Zhou, Y., and Van Roozendael, M.: Eight-component retrievals from ground-based MAX-DOAS observations, Atmos. Meas. Tech., 4, 1027–1044, https://doi.org/10.5194/amt-4-1027-2011, 2011.

[RD35:Irie2012] Irie, H., Boersma, K. F., Kanaya, Y., Takashima, H., Pan, X., and Wang, Z. F.: Quantitative bias estimates for tropospheric $NO_2$ columns retrieved from SCIAMACHY, OMI, and GOME-2 using a common standard for East Asia, Atmos. Meas. Tech., 5, 2403–2411, https://doi.org/10.5194/amt-5-2403-2012, 2012.

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# 3. User requirements

The climate data user requirements listed hereafter are reproduced from the Precursors_cci+ *User Requirements Document* [RD11:URD] and *The 2022 GCOS Implementation Plan* ([RD9:GCOS_IP] and its supplement [RD10:GCOS_Req]). Data format and metadata conventions outlined in the *CCI Data Standards* document are considered as well [RD19:CCI_standard].

## 3.1. URD requirements from user survey

The Precursors_cci+ URD [RD11:URD] outlines user requirements determined from the user survey conducted at the beginning of the project. The requirements were collected per ECV, but often reoccurred for different ECVs and/or are not product specific. Table 1 is a synthesis that identifies those that are within the scope of a validation. A detailed study of the documentation is out of scope; only the availability of documentation will be checked.

**Table 1. Summary of requirements collected from the user survey, adapted from [RD11:URD].**

| REQUIREMENT | PRODUCT TYPE | SOURCE IN URD |
|---|---|---|
| ***Documentation*** | | |
| Product User Manual (PUM) | L2, L3 | rec-NH3-1 |
| Algorithm Theoretical Basis Document (ATBD) | L2, L3 | rec-NH3-1 |
| Short readme on data product + how-to:<br>• quality filtering<br>• uncertainty when combining data<br>• application averaging kernel | L2, L3 | rec-SO2-1, rec-HCHO-1, rec-NO2-3, rec-NO2-2 |
| ***Data requirements*** | | |
| Pre-filtered data | L2 | rec-NH3-3 |
| Temporal sampling: daily and monthly | L3 | rec-HCHO-3, rec-NO2-2 |
| Consistent & stable | Multi-mission | rec-SO2-2 |
| ***Flags, auxiliary information*** | | |
| Quality flags | L2 | rec-NH3-3, rec-CHOCHO-1 |
| Snow/ice flags | L2 | rec-SO2-3 |
| Aerosol/Particle Matter flag | L2 NH3 | rec-NH3-3 |
| ***Uncertainty estimates*** | | |
| Uncertainty | L2, L3 | rec-SO2-4, rec-HCHO-3, rec-NO2-2 |
| Uncertainty budget<br>• random & systematic sources<br>• top two contributors | L2, L3 | rec-SO2-4<br>rec-NH3-3 |
| Vertical Averaging Kernel (AK) | L2, L3 | rec-SO2-4, rec-HCHO-3, rec-NH3-3, rec-CHOCHO-1 |
| A priori profile | L2 | rec-NH3-3, rec-CHOCHO-1 |
| Wind | L2 | rec-SO2-3 |
| Emissivity or similar | L2 NH3 | rec-NH3-3 |
| Fractional cloud cover | L2, L3 | rec-HCHO-3 |
| Surface properties | L2, L3 | rec-HCHO-3 |

## 3.2. Numerical quality requirements in 2022 GCOS IP and in URD

### 3.2.1. Generalities

The *2022 GCOS Implementation Plan* [RD10:GCOS_Req] defines five categories of requirements applicable generically to all ECVs:

1. **Spatial Resolution** - horizontal and vertical (if needed).
2. **Temporal resolution (or frequency)** – the frequency of observations, e.g., hourly, daily or annual.
3. **Measurement Uncertainty** – the parameter, associated with the result of a measurement, that characterizes the dispersion of the values that could reasonably be attributed to the measurand [RD14:GUM]. It includes all contributions to the uncertainty, expressed in units of 2 standard deviations, unless stated otherwise.
4. **Stability** – The change in bias over time. Stability is quoted per decade.
5. **Timeliness** - The time expectation for accessibility and availability of data.

For each of these categories, a *goal*, *breakthrough* and *threshold* value are presented. These are defined in the *2022 GCOS Implementation Plan* as:

- **Goal (G)**: an ideal requirement above which further improvements are not necessary.
- **Breakthrough (B)**: an intermediate level between threshold and goal which, if achieved, would result in a significant improvement for the targeted application. The breakthrough value may also indicate the level at which specified uses within climate monitoring become possible. It may be appropriate to have different breakthrough values for different uses.
- **Threshold (T)**: the minimum requirement to be met to ensure that data are useful.

The *2022 GCOS Implementation Plan* assigns a numerical value to these data quality requirements for the (tropospheric) column of $NO_2$, HCHO, $SO_2$ and CO, but not for $NH_3$ and CHOCHO. To circumvent this omission, the Precursors_cci+ project consortium has proposed 'GCOS-equivalent' requirements [RD11:URD] determined after a dedicated user consultation.

### 3.2.2. Tropospheric nitrogen dioxide column

$NO_2$ data product requirements are reproduced from [RD10:GCOS_Req]. These also served as input to [RD11:URD]. It is usual practice to express uncertainty in 1-sigma, therefore the table is adapted accordingly.

**Table 2. 2022 GCOS IP requirements for the ECV tropospheric $NO_2$ column, adapted from [RD10:GCOS_Req]. Specifically, 2-sigma uncertainty is adapted to 1-sigma.**

| QUANTITY | THRESHOLD | BREAKTHROUGH | GOAL |
|---|---|---|---|
| Horizontal resolution | 100 km | 30 km | 10 km |
| Vertical resolution | N/A | N/A | N/A |
| Temporal resolution | 30 days | 1 day | 1 hour |
| Timeliness | 30 days | 7 days | 1 day |
| Measurement uncertainty (1-sigma) | Max(50%, 2.5E15 molec $cm^{-2}$) | Max(20%, 1E15 molec $cm^{-2}$) | Max(10%, 0.5E15 molec $cm^{-2}$) |
| Stability | Max(20%, 1E15 molec $cm^{-2}$/decade) | Max(8%, 1E15 molec $cm^{-2}$/decade) | Max(4%, 1E15 molec $cm^{-2}$/decade) |

The absolute (relative) requirement on measurement uncertainty is applicable below (above) measurand values of 5E15 molec $cm^{-2}$.

### 3.2.3. Tropospheric formaldehyde column

HCHO data product requirements are reproduced from [RD10:GCOS_Req]. These also served as input to [RD11:URD]. It is usual practice to express uncertainty in 1-sigma, therefore the table is adapted accordingly.

**Table 3-3. 2022 GCOS IP requirements for the ECV tropospheric HCHO column, adapted from [RD10:GCOS_Req]. Specifically, 2-sigma uncertainty is adapted to 1-sigma.**

| QUANTITY | THRESHOLD | BREAKTHROUGH | GOAL |
|---|---|---|---|
| Horizontal resolution | 100 km | 30 km | 10 km |
| Vertical resolution | N/A | N/A | N/A |
| Temporal resolution | 30 days | 1 day | 1 hour |
| Timeliness | 30 days | 7 days | 1 day |
| Measurement uncertainty (1-sigma) | Max(50%, 20E15 molec $cm^{-2}$) | Max(20%, 8E15 molec $cm^{-2}$) | Max(10%, 4E15 molec $cm^{-2}$) |
| Stability | Max(20%, 8E15 molec $cm^{-2}$/decade) | Max(8%, 8E15 molec $cm^{-2}$/decade) | Max(4%, 8E15 molec $cm^{-2}$/decade) |

The absolute (relative) requirement on measurement uncertainty is applicable below (above) measurand values of 40E15 molec $cm^{-2}$.

### 3.2.4. Tropospheric sulphur dioxide column

$SO_2$ data product requirements are reproduced from [RD10:GCOS_Req]. These also served as input to [RD11:URD]. It is usual practice to express uncertainty in 1-sigma, therefore the table is adapted accordingly.

**Table 3-4. 2022 GCOS IP requirements for the ECV tropospheric $SO_2$ column, adapted from [RD10:GCOS_Req]. Specifically, molec cm-2 is adapted to DU and 2-sigma uncertainty to 1-sigma.**

| QUANTITY | THRESHOLD | BREAKTHROUGH | GOAL |
|---|---|---|---|
| Horizontal resolution | 100 km | 30 km | 10 km |
| Vertical resolution | N/A | N/A | N/A |
| Temporal resolution | 30 days | 1 day | 1 hour |
| Timeliness | 30 days | 7 days | 1 day |
| Measurement uncertainty (1-sigma) | Max(50%, 0.37 DU) | Max(30%, 0.22 DU) | Max(15%, 0.11 DU) |
| Stability | Max(20%, 0.15 DU/decade) | Max(12%, 0.089 DU/decade) | Max(6%, 0.045 molec $cm^{-2}$/decade) |

The absolute (relative) requirement on measurement uncertainty is applicable below (above) measurand values of 0.73 DU.

### 3.2.5. Tropospheric carbon monoxide column

CO data product requirements are reproduced here from [RD10:GCOS_Req]. These also served as input to [RD11:URD]. It is usual practice to express uncertainty in 1-sigma, therefore the table is adapted accordingly.

**Table 3-5. 2022 GCOS IP requirements for the ECV tropospheric CO column, adapted from [RD10:GCOS_Req]. Specifically, 2-sigma uncertainty is adapted to 1-sigma.**

| QUANTITY | THRESHOLD | BREAKTHROUGH | GOAL |
|---|---|---|---|
| Horizontal resolution | 100 km | 30 km | 10 km |
| Vertical resolution | N/A | N/A | N/A |
| Temporal resolution | 30 days | 1 day | 1 hour |
| Timeliness | 30 days | 7 days | 1 day |
| Measurement uncertainty (1-sigma) | 5 ppb | 2.5 ppb | 0.5 ppb |
| Stability | 2 ppb/decade | 1 ppb/decade | <1 ppb/decade |

### 3.2.6. Tropospheric ammonia column

At the time of writing, no GCOS requirements were formulated for $NH_3$ column products, therefore requirements were formulated in [RD11:URD]. $NH_3$ data product requirements are reproduced here from [RD11:URD]. It is usual practice to express uncertainty in 1-sigma, therefore the table is adapted accordingly.

**Table 3-6. Consortium specified user requirements for $NH_3$ tropospheric column, adapted from the URD [RD11:URD]. Specifically, 2-sigma uncertainty is adapted to 1-sigma.**

| QUANTITY | THRESHOLD | GOAL |
|---|---|---|
| Horizontal resolution | 100 km | 10 km |
| Vertical resolution | N/A | N/A |
| Temporal resolution | 1 week | 1 hour |
| Measurement uncertainty (1-sigma) | Max(50%, 5E15 molec $cm^{-2}$) | Max(20%, 1.25E15 molec $cm^{-2}$) |
| Stability | Max(10%, 2e+15 molec. $cm^{-2}$ /decade) | Max(2%, 1e+15 molec. $cm^{-2}$ /decade) |

The absolute (relative) threshold requirement on measurement uncertainty is applicable below (above) measurand values of 10E15 molec $cm^{-2}$. The absolute (relative) goal requirement on measurement uncertainty holds below (above) measurand values of 6.25E15 molec $cm^{-2}$.

### 3.2.7. Tropospheric glyoxal column

At the time of writing, no GCOS requirements were formulated for $NH_3$ column products, therefore requirements were formulated in [RD11:URD]. Glyoxal data product requirements are reproduced here from [RD11:URD]. It is usual practice to express uncertainty in 1-sigma, therefore the table is adapted accordingly.

**Table 7. Consortium specified user requirements for glyoxal tropospheric column, from the URD [RD11:URD].**

| QUANTITY | THRESHOLD | GOAL |
|---|---|---|

| | | |
|---|---|---|
| Horizontal resolution | 100 km | 10 km |
| Vertical resolution | N/A | N/A |
| Temporal resolution | 30 days | 1 hour |
| Measurement uncertainty (2-sigma) | Max(25%, 2E14 molec $cm^{-2}$) | Max(5%, 1E14 molec $cm^{-2}$) |
| Stability | Max(25%, 2e+14 molec. $cm^{-2}$ /decade) | Max(10%, 1e+14 molec. $cm^{-2}$ /decade) |

The absolute (relative) threshold requirement on measurement uncertainty is applicable below (above) measurand values of 8E14 molec $cm^{-2}$. The absolute (relative) goal requirement on measurement uncertainty holds below (above) measurand values of 20E14 molec $cm^{-2}$.

## 3.3. Data format and metadata conventions

The baseline proposal declares that a main objective of the CCI+ project on ECV precursors is to 'Generate long time multi-mission series of level-2 and level-3 data records for the five Precursor variables using a common file format and harmonized metadata fields, in line with the guidelines for CDR data production defined by the CCI Data Engineering Working Group (DEWG)'.

The baseline proposal also requires that 'All data products generated in the project will adopt harmonized format and metadata structures following the CCI guidelines.' ([RD1:BP], sections 1.1.3.2 and 1.1.6). The latest version of the CCI guidelines available so far is the *CCI Data Standards* v2.3 document [RD19:CCI_standard].

These guidelines encompass, e.g., the structure of the filename, the data format (netCDF-4), naming conventions for top-level and variable attributes (taking from the netCDF-Climate and Forecasting conventions [RD18:CF]), and the internal file structure (no groups unless after discussion with the CCI Data Standards team).

# 4. ECV Data Product Validation Protocol

## 4.1. Generic principles applicable to all ECVs

### 4.1.1. Validation protocol for atmospheric composition satellites

The generic validation protocol adopted here, was designed for the round-robin evaluation of satellite nadir ozone profiling, and first published and applied to MetOp-A GOME-2 ozone profiles in [RD48:Keppens2015] (see Figure 1 for an update). Several of its principles were adopted in the generic validation practices across EO domains published in 2017 by [RD47:crossEOval] and further formalised in ISO/TS 19124-1:2023. Discussed in the Ozone_cci+ project, and reported at plenary meetings of the CEOS WG on Cal/Val (WGCV) and the CEOS Atmospheric Composition Constellation (AC-VC), this protocol was extended in [RD50:Compernolle2016] and [RD51:Compernolle2018] for the validation of ECV precursors $NO_2$, HCHO and CO CDRs in the context of the EC FP7 QA4ECV project. Since, it has been applied in a long list of studies and activities, including the ground-based validation of ozone CDRs produced as an outcome of the ESA Ozone_cci projects and the ECMWF/C3S ozone product procurement service, and the operational validation of the Sentinel-5p TROPOMI trace gas data products carried out in the ESA/Copernicus Atmospheric Missions Mission Performance Cluster (ATM-MPC).

Base on this heritage, the validation protocol that will be applied to the ECV precursors CDRs generated in the Precursors_cci+ project is divided into the 10 steps described in Table 8 and illustrated in Figure 1.

**Table 8. Validation protocol for the satellite-based Climate Data Records of ECV precursors**

| STEP | PROCESS |
|---|---|
| 1 | Translation of data user requirements into validation requirements. |
| 2 | Selection, filtering and post-processing of satellite-based CDRs and of reference datasets. |
| 3 | Data content study of satellite-based ECV CDRs. |
| 4 | Information content study of satellite-based ECV CDRs. |
| 5 | Set-up and application of data co-location process (between satellite CDRs and reference datasets). |
| 6 | Identification and characterization of co-located data pairs. |
| 7 | Data harmonization processes: quantity, vertical grid, vertical smoothing… |
| 8 | Data comparison process and production of statistical estimates. |
| 9 | Derivation of Quality Indicators: bias, dispersion, stability, resolution… |
| 10 | Production of user-oriented report, including an overview of Quality Indicators and the evaluation of CDR data quality compliance with respect to 2022 GCOS IP and other URD data user requirements. |

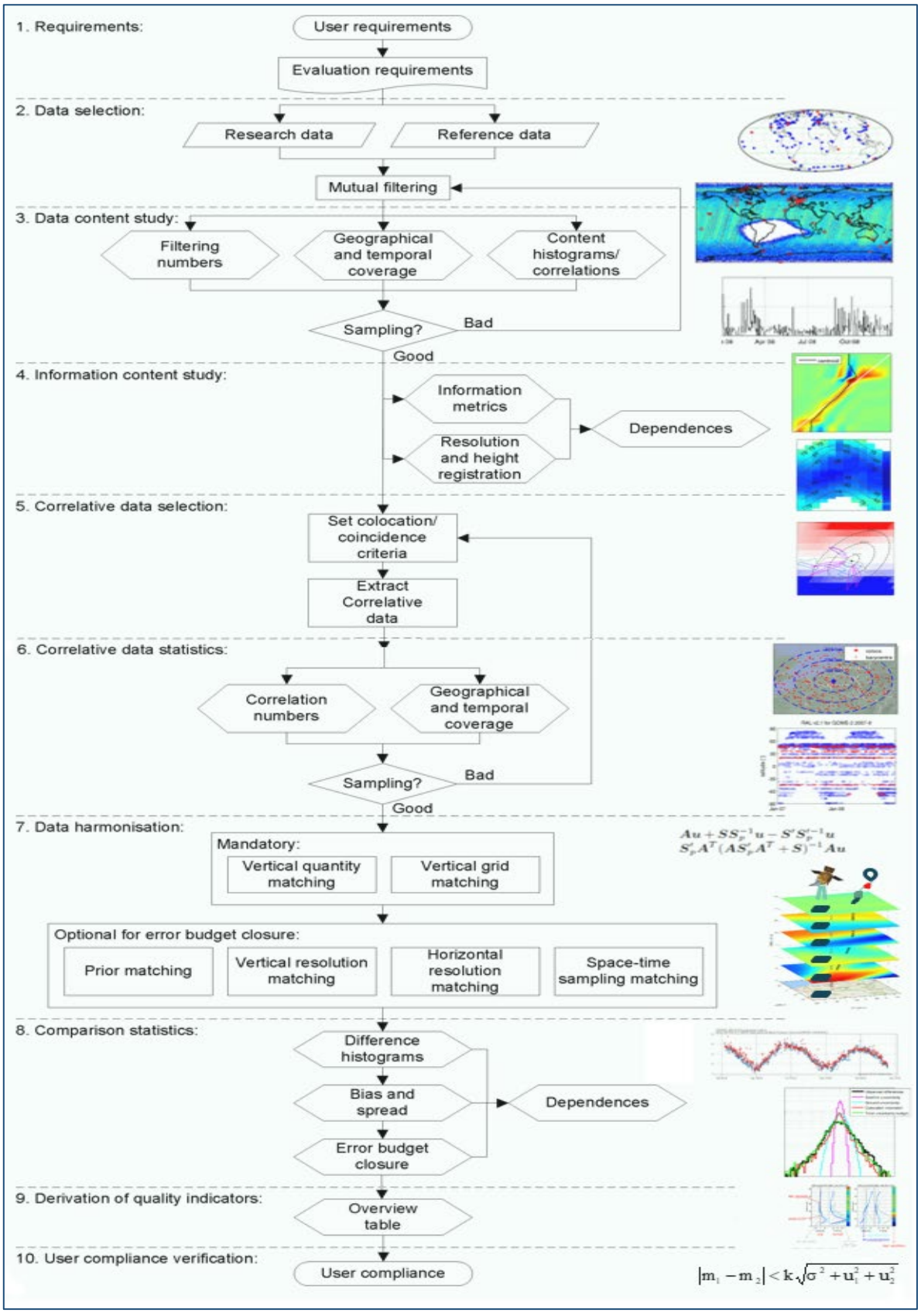



**Figure 1. Generic validation and round-robin protocol for satellite-based remote sensing data of atmospheric composition, updated from [RD48:Keppens2015].**

Note that depending on the data product, the quality of the available reference measurements and the scope of the validation, some steps might not always be applicable, e.g., the information content study in absence of Averaging Kernels.

The user requirements themselves are collected in Section 3 of the present document, and their translation into validation requirements (**Step 1** of the validation protocol) later in this Section 4.1. As it is not yet fully decided how the satellite data sets will be made available, the selection of satellite data (**Step 2**) cannot be made concrete yet. In any case, quality filtering as recommended by the data provider will be applied. Step 2 also includes bunch collection of the reference data, prior to their finer selection and co-location foreseen later in Step 5. This aspect is described initially in Section 5, with refinements foreseen in the course of the project.

Part of the compliance of the CDR quality with respect to user requirements can be checked with a Data Content Study and, if applicable, with an Information Content Study (**Steps 3 and 4** of the validation protocol) of the satellite data. Such studies are described in the general and specific parts of Section 4.

To check some other user requirements, Quality Indicators have to be generated using reference data. The collection and characterization of reference data is **Step 5** of the validation protocol. High-level characterization of these reference data can be found in Section 5, with practical details on data access and data policy in Section 5.2.

Details on **Steps 6 to 8** are highly dependent on the satellite product type (e.g., ECV-type, horizontal resolution) and the type of reference measurement.

The derivation of quality indicators (**Step 9**) will be based on the validation metrics specified in Section 4.1.4.

In **Step 10**, the user-oriented report will be the Precursors_cci+ *Product Validation and Intercomparison Report* (PVIR), a major deliverable of the project. This report will include an assessment of the level of compliance of each produced satellite-based CDR with respect to *The 2022 GCOS Implementation Plan* and other data user requirements. Note that not only the main geophysical variables (vertical column density), but also their reported uncertainties and the associated flags and data usage recommendations will be checked.

### 4.1.2. Maturity assessment of satellite data validation

To evaluate the maturity of any Earth Observation dataset, the CEOS WGISS has developed the *Data Management and Stewardship Maturity Matrix* (DMSMM) [RD17:WGIS_MM]. This evaluation system includes the field 'Data Validation' for the assessment of four major aspects of the validation carried out on the data product (MMP-6 component of DMSMM). Table 9 reproduces the maturity criteria for this component that will be applied in the Precursors_cci+ project.

**Table 9. Maturity criteria from the WGISS Data Management and Stewardship Maturity Matrix [RD17:WGIS_MM], for the component 'Data Validation' (MMP6).**

| 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. |

### 4.1.3. Validation against user requirements

User requirements are defined in the URD [RD11:URD] and the *2022 GCOS Implementation Plan* [RD10:GCOS_Req], on which summary tables reproduced in Section 3 are based. As seen in section 4.1.1, Step 1 of the validation protocol consists in the translation of these user requirements into validation requirements. The last Step 10 of the validation protocol is to verify the level of compliance of the produced ECV CDRs against the data user requirements.

Compliance with the following user requirements will be checked from the outcome of the Data Content Study (Step 3 of the validation protocol in Table 8)

- Compliance with user requirements such as availability of auxiliary data, averaging kernels, uncertainty and uncertainty components (see Table 1), … can be done by simple inspection of the product specifications and/or file content checks.
- Also product specifications and/or file content checks, the file **data format and metadata** can be compared to the CCI Data Standard [RD19:CCI_standard], see Section 3.3. However, a full assessment of compliance of data format and metadata according to the CCI Data Standard is out of scope. The focus will be on those fields with clear links to the user requirements.
- Time series will be visualized. This allows to check the **consistency** (see Table 1) of the multi-sensor CDRs (e.g., to detect artefacts caused by the combination of multiple sensors).
- Assessment of compliance with requirements on **observation frequency** and **spatial resolution** is straightforward. The product specifications can be directly compared to the user requirements.

By confrontation with independent reference data, also the following requirements can be tested.

- Compliance with requirements on **total uncertainty** can be verified by classical comparisons yielding bias and dispersion estimates and combined metrics like the RMSD (generated in step 9), taking into account comparison error and reference uncertainty terms.
- To estimate the **decadal stability**, the temporal trend of the bias is to be calculated. The method of Hubert et al., (2016) [RD78:Hubert2016] and/or [RD79:Vigouroux2015] will be applied, which produces robust estimates with weak influence of outliers. A multiple linear regression can be applied to separate the drift from the seasonal cycle (See further in 4.1.5)
- Where possible, validation metrics based on comparisons between satellite and reference data should be calculated **without and with application of the averaging kernel** to the reference profile (e.g., Rodgers and Connor, 2003 [RD76:Rodgers2003]), as some users want to minimize the dependence between the satellite retrieval settings (in particular the prior profile shape) and their application of interest (e.g., comparison with models). The application of the averaging kernel is a kind of data homogenization (Step 7 of the validation protocol)

### 4.1.4. Validation metrics and their link with user requirements

Step 9 of the validation protocol refers to the generation of statistical quality indicators derived from the comparison of the satellite data with respect to the reference data. The specific validation metrics that will be used here, and which are used in e.g., [RD55:Compernolle2020][RD59:Vigouroux2020][RD54:Verhoelst2021], are presented in Table 10. Both robust and non-robust metrics are provided; combining both gives insight in the impact of outliers. Note that mean and standard deviation of the relative difference are not tabulated here as they can easily generate non-sensible results (e.g., due to a small denominator).

**Table 10. Specific validation metrics to be derived from the comparison to reference data**

| QUALITY INDICATOR | METRIC |
|---|---|
| bias | median(Δ), median(Δr)<br>mean(Δ) |
| dispersion | ½IP68(Δ), ½IP68(Δr)<br>std(Δ) |
| total uncertainty estimate<br>(encompassing systematic and random error) | RMS(Δ)=√[mean(Δ)$^2$+std(Δ)$^2$]<br>√[median(Δ)$^2$+½IP68(Δ)$^2$], √[median(Δr)$^2$+½IP68(Δr)$^2$] |
| stability | temporal trend of the bias, in percent per decade<br>E.g., robust method of Hubert et al., (2016) |
| proportional and constant bias | Theil-Sen slope and intercept |

Δ =SAT-REF. Δr =(SAT-REF)/REF [%]. REF can be both the original data, or the data after application of the averaging kernel. RMS: root-mean-square, which is equal to sqrt(mean(Δ)$^2$+std(Δ)$^2$). ½IP68: half of the difference between the 84 percentile and the 16 percentile. std: standard deviation.

Step 10 of the validation protocol is the evaluation of compliance of the CDR quality with user requirements. The 2022 GCOS IP requirement on total measurement uncertainty (value defined for two sigma) encompasses random and systematic errors, but a separate view on these two aspects is often desired. Therefore:

- It will be checked if the dispersion metrics are within 50% of the GCOS requirement value on measurement uncertainty. The factor of 50% is needed since the dispersion metrics in Table 1 correspond to one sigma, while the GCOS requirement value is for two sigma.
- It will be checked if the bias is within the requirement value on measurement uncertainty, at two-sigma (corresponding to 95% confidence interval) or 1-sigma (68% confidence interval; factor of 50% applied on the requirement value).
- It will be checked if the total uncertainty estimates are within the requirement on measurement uncertainty.
- It will be checked if the temporal trend of the bias is within the requirement value on stability.

To the extent possible, the contribution of reference data uncertainty and of comparison error to the validation metrics should be minimized or characterized (see also Section 5). It must be noted that, while efficient methods have been developed for this for species like ozone, their application to ECV precursors remains a challenge and a matter of research.

### 4.1.5. Tools and auxiliary data

For regular tasks (reading in data, co-location, data homogenization, plotting, ... ) in-house tools of the different research groups and/or the open source tool HARP [RD80:HARP] will be used.

For the validation of the satellite stratospheric NO2 column (in the mid-morning or early afternoon) with respect to ground-based ZSL-DOAS (at twilight), a photochemical correction will be applied for the solar local time difference between the measurements. The correction factor is calculated with the PSCBOX 1D stacked-box photochemical model [RD81:Errera2001][RD23:Hendrick2004]), initiated by daily fields from the SLIMCAT chemical transport model (CTM). This photochemical correction factor is an average based on 10 years of the box-model simulations, and its uncertainty is considered to be within 6% [RD54:Verhoelst2021].

To study the drift, a multiple linear regression (MLR) is applied on the time-series ***Y(t)*** of the absolute differences satellite-groundbased at each site. We prefer a multiple linear regression for cases where the biases show a strong seasonal dependency. So, a seasonal cycle (4 harmonics) is fitted together with the trend (or "drift") **B**:

$$Y(t)= a + \mathbf{B} * t + C_1 * \cos(2\pi * t) + C_2 * \sin(2\pi * t) + C_3 * \cos(4\pi * t) + C_4 * \sin(4\pi * t) \quad \text{(Eq.1)}$$

Note that to reduce the influence of outliers on the drift calculation, a robust multiple linear regression is used (bisquare method).

### 4.1.6. Validation of individual processing components

ECV line components are the individual processing blocks by which ECV data products are generated in their interim or final version. For complex processing chains, international standards require to validate or at least verify the good performance of every component and the accuracy of its output.

Limiting validation to the final data product only is not sufficient. The validation – or at least some relevant quality check – of intermediate data products is highly desirable to avoid, e.g., that the apparently good behaviour of the final data product at the end of the chain hides large compensating errors affecting separate components of the data retrieval.

For the round-robin studies, this will be accomplished in a limited way by comparison of the cloud height parameters of the candidate cloud processors (FRESCO and OCRA ROCINN) of the HCHO product with those of Cloudnet, and by comparison of the prior HCHO and SO2 profiles of the candidate models (TM5 and CAMS) with those of MAX-DOAS.

For the comprehensive validation of the final CDRs, this will be done for the $NO_2$ product, by the validation of the stratospheric $NO_2$ column, known as an important intermediate step in the retrieval of the tropospheric $NO_2$ column.

Similarly, the validation of the L2 products will be the grounding step of the validation of the L3 products (see Section 2.2.5.2) which are a main data deliverable of this project.

### 4.1.7. Error budget closure of a data comparison

A major objective of the ground-based validation is to assess the validity of the theoretical (ex-ante, or prognostic) uncertainty estimates provided in the satellite data product. However, the discrepancy between the satellite dataset being validated and the reference dataset combines uncertainties associated with each individual measurement system, plus uncertainties associated with the methodology of data comparison. Uncertainties associated with the comparison methodology include the following sources of co-location mismatch:

(i) Comparison uncertainties associated with the difference in sampling of atmospheric variability and structures: e.g., geographical mismatch, diurnal cycle effects, assumptions related to the area of representativeness.

(ii) Comparison uncertainties associated with the difference in smoothing of atmospheric variability and structures: e.g., MAX-DOAS measurements sampling an air mass of a few km long, compared with GOME ground pixels of 40 x 320 $km^2$ or TROPOMI ground pixels of 5.5 x 3.5 $km^2$.

As much as possible, comparison uncertainties due to co-location mismatch will be reduced by a cautious design of the selection of data sets to be compared, and by considering that a multivariate analysis of the comparison results taking into account the specifics of the data being compared (modelling data or remote sensing data, atmospheric variability and gradients etc.) might be required and preferred over entirely statistical approaches. For traceability purposes it is essential to document, for each validation exercise, the selection method applied to the data sets (temporal and spatial co-location criteria, how differences in vertical and horizontal smoothing are handled etc.) [RD77:Keppens2019].

Although essential, the closure of a complete error budget for each data comparison is still a matter of research at the time being [RD86:Verhoelst2015] and it falls partly beyond the scope of the Precursors_cci+ precursor project. Validation researchers as well as data producers are aware that neglecting uncertainties linked to the comparison method can yield erroneous conclusions on the quality of the compared data product. This awareness must be transmitted to the reader of Precursors_cci+ PVIR for a proper use of the validation results and, in fine, of the ozone precursor ECV data records. When misinterpretation is possible, common statements like “the discrepancy between the two data sets ranges within their individual error bars” will be suitably annexed with a provision on the – actual calculated or simply expected – contribution of the selection and comparison methods to this discrepancy. Provisions like “temporal and spatial mismatches exist but their contribution to the discrepancy between the two data sets has not been assessed; nevertheless, this contribution is assumed to be small…” or “the selection method has been optimised to reduce apparent discrepancies between the data products, that would be generated actually by temporal and spatial mismatches and by differences in smoothing of atmospheric variability” are acceptable examples.

The method of [RD83:Immler2010] will be used to qualify the agreement of the satellite and reference datasets, and the consistency of the combined error budget. Another method recently applied successfully to TROPOMI $O_3$ and $NO_2$ validation is the chi-square method [RD84:ROCVR].

### 4.1.8. Satellite data intercomparison

By definition (see Section 5.1.1), satellite data cannot be considered stricto sensu as an independent source of validation. Nevertheless, they are essential to extend ground-based validation to the global domain and be able to detect spatial patterns, temporal signals and other features not accessible by ground-based observation. Figure 2 shows that the number of sounders measuring the targeted ECV precursors is small, actually poorer than that for several other ECVs, and the planned Precursors_cci+ CRDP already include most of the sounders with state-of-the-art capabilities and/or access to the relevant level-1 and level-2 data. Therefore, the project cannot rely on extensive satellite data intercomparisons only.

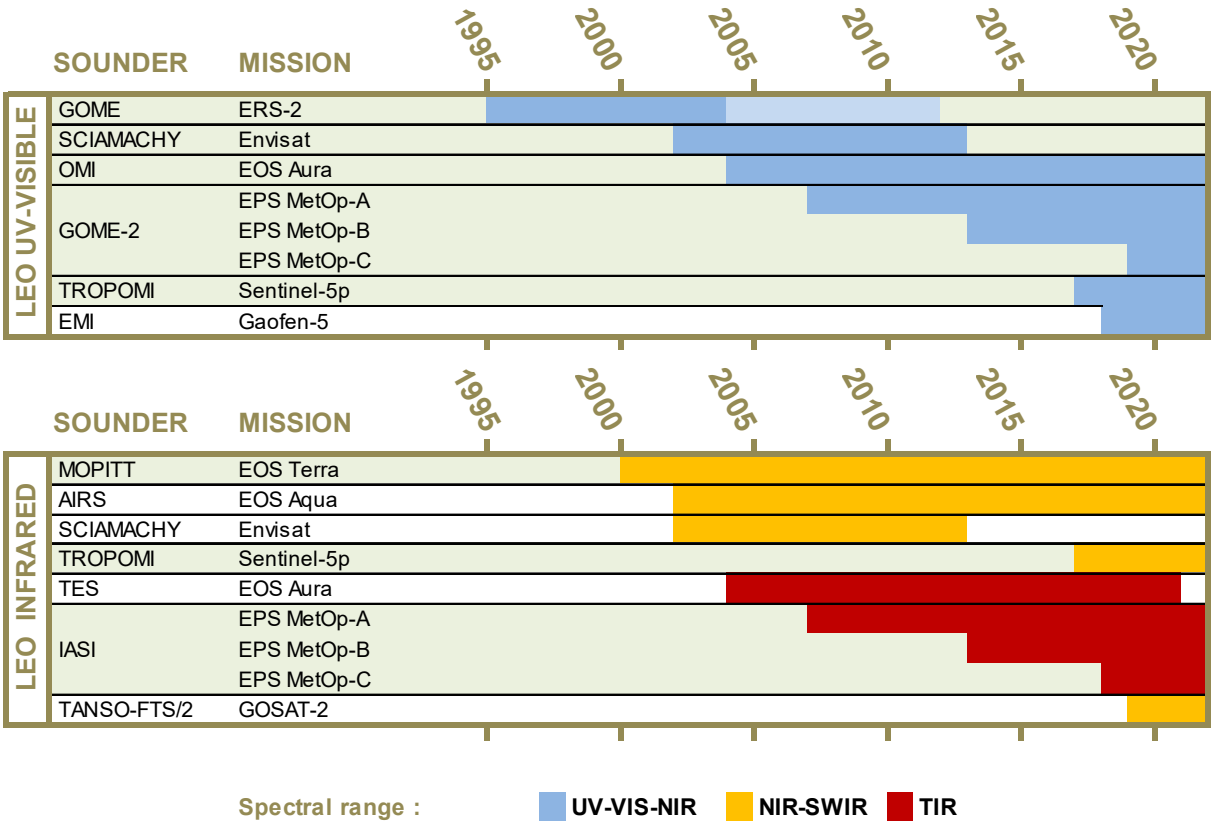



**Figure 2. Planning of UV-visible (top) and Infrared (bottom) nadir sounding missions measuring one or several of the ECV precursors targeted by this project. The main colour code identifies the spectral range of the sounder. Entries highlighted in green: missions planned to contribute to the CRDP. Entries in white: other missions not considered by the project.**

Satellite data intercomparisons will be carried out by data producers on an *ad hoc* basis for the following purposes:

- Satellite data in space and time overlap will be intercompared in the multi-sensor merging procedure to determine and correct for potential biases (see Section 4.1.9).
- Satellite data produced from the same sounder but processed with alternative algorithms will be intercompared as part of the round-robin studies (e.g., COBRA SO2 vs. DOAS and PCA, or QA4ECV NO2 vs STREAM NO2) and reported in [RD6:PVASR].

Quality information derived from these studies will be reported in the PVIR as appropriate (see e.g., [RD8:PVIRv2], for QA4ECV vs STREAM NO2.

### 4.1.9. Level-3 data validation

The Precursors_cci+ Climate Research Data Package (CRDP) includes Climate Data Records of level-3 nature, in the form of gridded monthly files. The aggregation of level-2 data into level-3 data propagates additional uncertainties and smoothing on top of the original level-2 uncertainties. The multi-sensor merging of data from several different satellites adds another layer of complexity and of uncertainty sources. As a consequence, level-2 validation results are rarely directly transferable to level-3 data, and level-3 data validation must consider the effects of these additional data manipulations. The adopted validation approach consists in five steps:

(i) Collection of level-2 data validation results and derived Quality Indicators, and identification of the known quality issues expected to propagate into the level-3 data.
(ii) Identification of the additional spatial and temporal signals that the level-3 generation process might have introduced in the datasets, including smoothing and sampling errors at small scales.
(iii) Where possible, conversion of the ground-based reference data records into level-3 like datasets, mimicking the level-2-to-3 data generation procedure as described in the Algorithm Theoretical Basis Documents (ATBD);
(iv) Comparisons of satellite-based and ground-based level-3 datasets with derivation of level-3 data Quality Indicators: bias, dispersion, cycles and long-term stability. The study of influence quantities like the solar zenith angle is obviously not applicable to aggregated data.
(v) Confrontation of level-3 derived Quality Indicators to level-2 derived Quality Indicators, with tentative interpretation of the reasons for the discrepancies between the level-3 and level-2 Quality Indicators.

Depending on the auxiliary data generated with the level-2-to-level-3 conversion process (representativeness, variability) that will be included in the level-3 data files, the level-3 validation can take different forms. Useful level-2-to- level-3 conversion auxiliary data are:

- the number or weight of observations per grid cell,

- representativeness metrics, e.g., the asymmetry and entropy parameters as defined by [RD82:Sofieva2014], and
- the variability of the observations within a grid cell (e.g., the standard deviation).

After iterating with data producers, the following variables have been included in the L3 NO2 and HCHO products: L3-specific quality assurance value, number of observations per grid cell, effective date and time (representativeness measure), standard deviation within the grid cell (variability measure).

With availability of the adequate level-2-to-3 conversion auxiliary data, the validation can follow the approach adopted by the Copernicus Climate Change Service (C3S) for the quality assurance of its satellite ozone data procurement (see C3S Ozone *Product Quality Assurance Document* [RD53:PQAD]). In the case of gridded monthly level-3 data, a good rule of practice is:

- Convert the ground-based data records into monthly averages.
- Keep only those monthly means with a specified minimum of representative ground-based observations.
- Co-locate spatially the ground-based monthly means with the corresponding satellite level-3 grid cell; co-locating the monthly means with the nearest cell centre coordinate is acceptable if the atmospheric field varies smoothly, otherwise the ground-based monthly means must be distributed over the cells intersecting an area representative of the measured ground-based air masses.
- Unless in excellent mutual agreement, data from multiple stations present in the same grid cell shouldn't be averaged, to not lose traceability.
- Keep only those monthly means where the ground-based effective day does not deviate a specified threshold from the satellite-based effective day (if that is provided) or from the month centre.

If the satellite standard deviation per grid cell is included in the level-3 data, one can additionally check the consistency of the individual ground-based observations with the probability density function generated using the satellite mean and standard deviation.

If representativeness parameters are provided in the level-3 product, the dependence of the difference (satellite minus reference) can be investigated in function of those parameters.

## 4.2. Validation specifics by ECV

### 4.2.1. Quantities with potential impact on ECV data quality

Table 11 outlines per satellite data product a list of parameters and quantities that have known potential effects on the data quality and against which the stability of the derived quality indicators shall be assessed. It is understood that, in addition to dependences on these parameters and quantities, the stability of the satellite data with respect to reference data will be checked over a space-time domain as comprehensive as possible, with due reporting of any detected dependence on latitude and season.

**Table 11. Retrieval parameters and influence quantities that have a known potential effect on the satellite data quality.**

| SATELLITE DATA PRODUCT | RETRIEVAL PARAMETER OR INFLUENCE QUANTITY |
|---|---|
| stratospheric NO2 VCD | solar zenith angle, cloud fraction, surface albedo |
| tropospheric VCD from UV-visible sounders: NO2, HCHO, SO2, CHOCHO | solar zenith angle, cloud fraction & cloud height, AOD*, AMF & clear-sky AMF*, surface albedo |
| tropospheric VCD from thermal infrared sounders (IASI and MOPITT): CO, NH3 | cloud properties, surface temperature, thermal contrast, a priori profile, viewing zenith angle |

*: this parameter might be not available in the satellite or reference data files.

### 4.2.2. Validation requirements common to all data products

For all data products, validation studies and resulting documentation will target the following aspects:

- Time series of the ECV data and of the main measurement and retrieval parameters with potential impact on the data quality (see Table 11) should be visualised, at least in a few representative ground-based stations. Any obvious quality issue like the frequent occurrence of outliers and unrealistic values should be detected, documented and filtered out appropriately before performing quantitative comparisons.
- Statistical estimators of the difference like the bias and the dispersion shall be calculated over different time periods and over different ranges of relevant parameters as listed below. In case of frequent occurrence of outliers, median and interpercentile values shall be preferred over mean and standard deviation values as they reduce the influence of outliers. Calculation of mean values and the associated standard deviation is nevertheless encouraged. In case of doubt, histograms of the relative difference might be helpful in determining the validity of statistical estimators.
- In the treatment of statistics, care will be given to disentangle as far as possible the different sources of ECV uncertainty and avoid misleading cancellation of mutually compensating errors. In particular, the dependence of the ECV data quality on main measurement and retrieval parameters (see Table 11) shall be investigated.
- Decadal stability of the bias shall be assessed and expressed in %/decade.
- Shorter term stability of the bias and dispersion shall be assessed, including annual cycle, interannual variability and shorter term variability of the bias.

### 4.2.3. Tropospheric $NO_2$ data product

#### 4.2.3.1. Validation requirements

In addition to the validation requirements specified in section 4.2.2, validation studies and resulting documentation will address the following targets:

- The intermediate product stratospheric NO2 column, as well as the end products tropospheric NO2 column and total NO2 column shall be validated.
- Where reference profile information is available, satellite averaging kernels will be applied to assess the impact of the vertical smoothing error.
- For tropospheric and total NO2, studies shall be carried out at least in 3 regimes: low pollution level, moderate pollution level and high pollution level.
- For stratospheric NO2, studies shall be carried out in three geographical zones, in both hemispheres: tropics, middle latitudes and polar areas. Higher meridian and regional sampling is encouraged where possible.

#### 4.2.3.2. Validation data sources

Section 5 describes the reference measurements to be used for validation studies and/or for cross-comparison studies, with details on their access. The following measurement data sets will be used:

- Ground-based $NO_2$ column measurements by ZSL-DOAS instruments, for the validation of the intermediate retrieval product stratospheric NO2 column.
- Ground-based tropospheric column and, where available, profile, NO2 measurements by MAX-DOAS, for the validation of the end retrieval product tropospheric NO2 column.
- Ground-based total column NO2 measurements by Pandora, for the validation of the end retrieval product total NO2 column.

#### 4.2.3.3. Maturity of Data Validation

Table 12 applies the DMSMM criteria to the validation of stratospheric NO2 VCD using ZSL-DOAS. The last field on ‘validation results’ can only be assessed after they are generated, which will be done in the PVIR.

**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* |

### 4.2.4. Tropospheric HCHO data product

#### 4.2.4.1. Validation requirements

In addition to the validation requirements specified in section 4.2.2, validation studies and resulting documentation will address the following targets:

- Where reference profile information is available, satellite averaging kernels will be applied to assess the impact of the vertical smoothing error.
- Studies shall be carried out at least in 3 regimes: low HCHO level, moderate HCHO level and high HCHO level.

#### 4.2.4.2. Validation data sources

Section 5 describes the reference measurements to be used for validation studies and/or for cross-comparison studies, with details on their access. The following measurement data sets will be used:

- Ground-based lidar/radar measurements by ACTRIS-Cloudnet, for the delta-validation of candidate cloud parameters used as input in the HCHO column retrieval. Cloudnet data has been adapted to and used as a reference for the HCHO round-robin studies, and can be re-used in future Precursors_cci+ related work, also for other Precursors_cci products than HCHO.
- Ground-based tropospheric column and profile HCHO measurements by NDACC FTIR, for the validation of the end retrieval product tropospheric HCHO column.
- Ground-based tropospheric column and, where available, profile, HCHO measurements by MAX-DOAS (NDACC and other sources), for the validation of the end retrieval product tropospheric HCHO column. Profile HCHO measurements will also be used for the delta-validation of candidate prior profile models as part of the round-robin.

### 4.2.5. Tropospheric $SO_2$ data product

#### 4.2.5.1. Validation requirements

In addition to the validation requirements specified in section 4.2.2, validation studies and resulting documentation will address the following targets:

- Where reference profile information is available, satellite averaging kernels will be applied to assess the impact of the vertical smoothing error.
- Studies shall be carried out for scenes dominated by anthropogenic pollution and dominated by volcanic pollution.

#### 4.2.5.2. Validation data sources

Section 5 describes the reference measurements to be used for validation studies and/or for cross-comparison studies, with details on their access. The following measurement data sets will be used:

- Ground-based tropospheric column and, where available, profile, SO2 measurements by MAX-DOAS, for the validation of the end retrieval product tropospheric SO2 column. Profile SO2 measurements will also be used for the delta-validation of candidate prior profile models as part of the round-robin.
- Ground-based total column SO2 measurements by direct-Sun DOAS Pandora instruments, for the validation of the end retrieval product SO2 column.

#### 4.2.5.3. Maturity of Data Validation

Table 13 applies the DMSMM criteria to the validation of tropospheric SO2 VCD using PGN Pandora data. The low value for maturity of reference data representativeness reflects the scarcity of reference data temporally and geographically.

**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* |

### 4.2.6. Tropospheric CO data product

#### 4.2.6.1. Validation requirements

In addition to the validation requirements specified in section 4.2.2, validation studies and resulting documentation will address the following targets:

- Where reference profile information is available, satellite averaging kernels will be applied to assess the impact of the vertical smoothing error.

#### 4.2.6.2. Validation data sources

Section 5 describes the reference measurements to be used for validation studies and/or for cross-comparison studies, with details on their access. The following measurement data sets will be used:

- Ground-based tropospheric column and profile CO measurements by NDACC FTIR, for the validation of the end retrieval product tropospheric CO column.
- Ground-based dry-air column-averaged mole fractions (XCO) from TCCON.

### 4.2.7. $NH_3$ data product

#### 4.2.7.1. Validation requirements

The validation requirements are those specified in section 4.2.2.

#### 4.2.7.2. Validation data sources

Section 5 describes the reference measurements to be used for validation studies and/or for cross-comparison studies, with details on their access. The following measurement data sets will be used:

- Ground-based tropospheric column NH3 measurements by FTIR, for the validation of the end retrieval product NH3 column.

### 4.2.8. CHOCHO data product

#### 4.2.8.1. Validation requirements

In addition to the validation requirements specified in 4.2.2, validation studies and resulting documentation will address the following targets:

- Where reference profile information is available, satellite averaging kernels will be applied to assess the impact of the vertical smoothing error.

#### 4.2.8.2. Validation data sources

Section 5 describes the reference measurements to be used for validation studies and/or for cross-comparison studies, with details on their access. The following measurement data sets will be used:

- Ground-based tropospheric column and, where available, profile, CHOCHO measurements by MAX-DOAS, for the validation of the end retrieval product tropospheric CHOCHO column.

### 4.2.9. Validation approach to data from geostationary missions

#### 4.2.9.1. Validation needs

The CEOS Atmospheric Composition Virtual Constellation (AC-VC) and the CEOS Working Group on Calibration and Validation / Atmospheric Compsotion Sub Group (WGCV-ACSG) formulated additional challenges specific to the validation of GEO AQ missions [RD67:CEOS_GEO-AQ-Val]. We present these in short here below.

1. Sampling of the diurnal cycle is a new key feature with respect to LEO. It needs to be demonstrated that temporally varying biases do not dominate the true diurnal variations.
2. Due to the strong daily variation of solar illumination and viewing geometries of GEO, diurnal cycle observations are sensitive to directional characteristics of clouds, aerosols, surface reflectance and orography. Availability of this information is particularly important.
3. Due to the improved horizontal resolution, mismatches of spatial representativeness near strong spatial gradients, and shadow effects due to clouds or orography in neighbouring pixels become particularly important.
4. Where different GEOs do not overlap, LEO and ground-based networks can serve as transfer standard.
5. Obtaining accurate geolocation is challenging for GEO and therefore needs to be validated.
6. As the satellite vertical sensitivity varies and the vertical distribution can strongly vary during the day, information on the vertical distribution is particularly important.

#### 4.2.9.2. Recommendation on time range to be processed

GEMS operational data is available from 2022/11 onwards. GIIRS-B was operational since 2022/04/12 until 2024/01/31, then relocated in 2024/02 and again operational since 2024/02/27, but with a modified spatial data coverage, covering less of Japan.

According to the extension proposal[RD3:EP], a single year of GEMS and GIIRS-B will be processed (L2 and L3). FRM availability depends on the year. According to FRM availability (see later), and assuming that the provider chooses to process from January to December, we propose:

- 2022 for GEMS NO2, as a compromise in PGN NO2 and MAX-DOAS NO2 availability. In 2021 PGN availability is relatively low, while MAX-DOAS availability is strongly reduced since 2023.
- 2021 or 2022 for GEMS HCHO regarding FTIR and MAX-DOAS HCHO availability. There is very low MAX-DOAS availability in 2023 or later.
- 2023 for GIIRS CO. GIIRS does not cover fully 2022, and due to the relocation since 2024/02 the Japanese Tsukuba station might be out of the spatial coverage.
- 2023 for GIIRS NH3, for the same reason. Note that the Hefei and Tsukuba FRM data have to be requested from the PIs. If the processed year does not have to start January 1, 2022/05/01 to 2023/04/30 would be an improved option, as more data is already available then.

Obviously, processing of more than one year of data is highly desired.

#### 4.2.9.3. Planned work

- As said in [RD3:EP], given the resources only L2 or L3 will be validated, not both. L2 validation is preferred as it allows a more detailed view and the data can be expected to be earlier available within the project.
- Note that as only 1 year will be available, drift assessment is outside the scope of the planned GEO validation.
- See section 4.2.2 and following for metrics and plots (e.g., time series) not specific for GEO.
- To validate the observed diurnal cycle (CEOS challenge 1), we need FRM data throughout the day. The MAX-DOAS, Pandora and FTIR are therefore well suited. The co-located column measurements of SAT, GB and their difference will be mapped to a single day, possibly split per season if the amount of data is sufficient.
- The validation metrics for bias, dispersion and total uncertainty, aggregated over the different stations, will also be calculated for the different solar local times of the day. A similar strategy was applied by [RD69:Ghahremanloo2025].
- While obtaining directional characteristics of clouds, surface reflectance and orography (CEOS challenge 2) is out of scope, we will check the QI dependence simultaneously on cloud parameters and SZA or VZA, to check if the cloud dependency varies with sun or instrument angle.
- Near the edges of the FOV of the GEO the viewing zenith angle reaches more extreme values, which could affect measurement quality. Depending on the spatial scope of the ground-based network, the QI can be evaluated at the different stations ifo VZA or station latitude & longitude.

- Well validated LEO should be used as a transfer standard between the different GEO measurement areas (CEOS challenge 4). Comparisons of GEMS (operational product) vs S5P\TROPOMI have indeed already proven their use in e.g., revealing latitudinally depending biases (see PEGASOS reports). To the extent possible, we will re-use GEO vs LEO analyses made by the data providers to complete the Precursors_cci+ PVIR with satellite cross-validation results, like e.g. L3 spatial maps of the ECV value difference to reveal spatially varying biases, and L3 latitude-time maps of the same difference to visualize cycles and other temporal patterns (see ROCVR#29).

# 5. Reference measurements

This section describes and reports an initial evaluation of the ground-based measurements to be used as a reference for the CDR validation tasks. It first introduces to the definitions of what constitutes a Fiducial Reference Measurement (FRM) and it identifies associated maturity criteria for the candidate reference datasets and their data uncertainty. Then, for each envisaged network of candidate measurement the data access and policy are described. Finally, the specific reference data sources are described.

The derivation of quality indicators relies mainly on comparisons against Fiducial Reference Measurements (FRM), that is, independent ground-based measurements of documented quality traceable to community-endorsed standards and suitable for satellite validation. Table 14 identifies by ECV the ground-based data planned to be used as a reference for the validation of the ECV Climate Data Records (CDR) to be generated by the project and for the round-robin studies (RR) intended to improve the retrieval algorithms.

**Table 14. Satellite-based ECV data products to be validated and the corresponding ground-based measurements planned to be used as a reference for the validation of the Climate Data Records (CDR) and for round-robin studies (RR), as specified in [RD1:BP].**

| ATMOSPHERIC OZONE AND AEROSOL ECV PRECURSOR | GEOPHYSICAL QUANTITY | GROUND-BASED REFERENCE MEASUREMENT |
|---|---|---|
| Nitrogen dioxide ($NO_2$) | Tropospheric $NO_2$ VCD | MAX-DOAS $NO_2$ profile<br>MAX-DOAS $NO_2$ tropo. VCD |
| | Stratospheric $NO_2$ VCD | ZSL-DOAS $NO_2$ VCD |
| | Total $NO_2$ VCD | PGN/Pandora $NO_2$ VCD |
| Formaldehyde (HCHO) | Tropospheric HCHO VCD | MAX-DOAS HCHO profile<br>MAX-DOAS HCHO tropo. VCD<br>FTIR HCHO profile & VCD |
| | HCHO prior profile (RR studies only) | MAX-DOAS HCHO profile |
| | Cloud height (RR studies only) | Cloudnet cloud height |
| Sulphur dioxide ($SO_2$) | $SO_2$ VCD | MAX-DOAS $SO_2$ tropo. VCD<br>PGN/Pandora $SO_2$ VCD |
| | $SO_2$ *a priori* profile (RR studies only) | MAX-DOAS $SO_2$ profile |
| Carbon monoxide (CO) | Tropospheric CO VCD | NDACC FTIR CO profile & VCD<br>TCCON FTIR CO VCD |
| Ammonia ($NH_3$) | Tropospheric $NH_3$ VCD | FTIR $NH_3$ profile & VCD |
| Glyoxal (CHOCHO) | Tropospheric CHOCHO VCD | MAX-DOAS CHOCHO profile<br>MAX-DOAS CHOCHO tropo. VCD |

## 5.1. Maturity of reference measurements

### 5.1.1. Maturity as a Fiducial Reference Measurement

Donlon and Zibordi define Fiducial Reference Measurements [RD16:FRM_def] as "*the suite of independent ground measurements that provide the maximum return on investment for a satellite mission by delivering, to users, the required confidence in data products, in the form of independent validation results and satellite measurement uncertainty estimation, over the entire end-to-end duration of a satellite mission.*" Therefore, FRM data must have associated with them demonstration of evidence of their exceptional traceability, accuracy, long-term stability, and cross-site consistency.

The following criteria are currently used to assess the FRM maturity of a candidate dataset:

1. FRM measurements should ideally have documented SI traceability using metrology standards and/or community recognised best practices;
2. FRM measurements are independent from the satellite geophysical retrieval process.
3. An uncertainty budget for all FRM instruments and derived measurements is available and maintained.
4. FRM measurement protocols, procedures and community-wide management practices (measurement, processing, archive, documents etc.) are defined, published openly and adhered to by FRM instrument deployments.
5. FRM are accessible to other researchers allowing independent verification of processing systems.
6. FRM measurements are acquired by fully characterized and regularly calibrated instruments assuring the best traceability, accuracy and stability.
7. FRM measurements are retrieved with state-of-the-art processing codes relying on the most up-to-date and community-accepted data reduction schemes.

Furthermore, the Committee on Earth Observation Satellites (CEOS) recommends that FRMs, as part of the Quality Assurance process for EO data, follow the principles and guidelines outlined in the GEO/CEOS Quality Assurance framework for Earth Observation (QA4EO). QA4EO states that "It is critical that all EO data and derived products are easily accessible in an open manner and have associated with them an indicator of their quality traceable to reference standards (preferably SI) to enable users to assess its suitability for their application, i.e., its "fitness for purpose"."

Using the defining characteristics of a FRM, the general requirements for the reference data can be assessed. This will be done using the following check-box.

**Table 15. Requirements for a FRM, following the definition of Donlon and Zibordi [RD16:FRM_def].**

| FRM CHARACTERISTIC | FULFILLED (YES/NO) | REMARK |
|---|---|---|
| Traceability to community-accepted standards and best practices | | |
| Independent from satellite measurement | | |
| Uncertainty budget | | |
| Community-accepted best practices<br>• measurement protocol<br>• processing<br>• archiving<br>• documentation<br>Defined, published openly, adhered to | | |
| Easily accessible | | |
| Fully characterized and regularly calibrated | | |
| State-of-the-art processing codes | | |
| FRM Quality indicator traceable to reference standards | | |
| FRM-derived Quality Indicator | | |

### 5.1.2. Maturity of associated uncertainty estimates

'Data Uncertainty' is component MMP7 of the WGISS *Data Management and Stewardship Maturity Matrix* (DMSMM), since "To ensure measurements are both meaningful and defensible it is crucial that they come with rigorously evaluated uncertainty estimates" [RD17:WGIS_MM]. The uncertainty estimates provided with the reference data will be assessed with respect to the DMSMM MMP7 criteria reproduced in Table 16.

**Table 16. Maturity criteria from the WGISS Data Management and Stewardship Maturity Matrix (DMSMM) , for the component Data Uncertainty (MMP7).**

| | 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. |

## 5.2. Data access and policy of ground-based monitoring networks

### 5.2.1. The Network for the Detection of Atmospheric Composition Change (NDACC)

The Network for the Detection of Atmospheric Composition Change (NDACC) provides the following ground-based data that can be used as a reference for this project:

- ZSL-DOAS UV-visible spectrometers: (stratospheric) $NO_2$ column,
- MAX-DOAS UV-visible spectrometers: tropospheric $NO_2$ and HCHO column/profile, and CHOCHO column,
- FTIR spectrometers: CO column/profile, and HCHO and $NH_3$ column.

The NDACC Data Host Facility (DHF) provides public access to the data, free of charge. Parts of the NDACC HDHF are mirrored to the ESA Atmospheric Validation Data Centre (EVDC). The NDACC Data Use Agreement defines guidelines for data access, use and publication (https://ndacc.larc.nasa.gov/data/use-agreement). Hereafter we reproduce elements of this Data Use Agreement which are of direct relevance to the CCI projects.

NDACC Data Use Agreement

**Data Use Agreement**

If the metadata of an NDACC data file contain an explicit Data License and/or explicit DATA_RULES_OF_USE, then the indicated Rules of Use prevail over the following General Rules of Use. In the absence of a Data License or explicit DATA_RULES_OF_USE associated with the datafile, the following General Rules of Use apply:

**General Rules of Use**

All NDACC data users at a minimum **should acknowledge** both the NDACC DHF and the NDACC PI in any publication, as follows:

**Mandatory acknowledgement:**

*"The data used in this publication were obtained from "NDACC PI name" as part of the Network for the Detection of Atmospheric Composition Change (NDACC) and are available through the NDACC website www.ndacc.org."*

When it is envisaged to use NDACC data in a publication or communication, the respective NDACC PI(s) or IWG co-chairs should be contacted during the preparation of the publication or communication to discuss possible collaboration with the NDACC PI and co-authorship.

**In all cases**, NDACC data users are expected to consult the online documentation and reference articles to fully understand the scope and limitations of the NDACC datasets available at the NDACC DHF. They are strongly encouraged to contact the respective NDACC PI (listed in the data documentation on the web page) to receive any additional information regarding the data product that could be useful in their studies/applications and as such ensure the proper use of specific data sets.

Last revised date
February 18, 2021

### 5.2.2. The Pandonia Global Network (PGN)

The Pandonia Global Network (PGN) of Pandora instruments provides the following ground-based data that can be used as a refernce for this project : total column $NO_2$ and total column $SO_2$. Public access is provided at https://www.pandonia-global-network.org, with the data in ASCII format. The data is also submitted to EVDC and stored there in HDF GEOMS format. It is the latter data collection that we use.
Hereafter we reproduce the PGN data use guidelines (https://www.pandonia-global-network.org/home/documents/pgn-data-use-guidelines/).

**PGN data use guidelines**

Latest change 8 Feb 2021

The PGN provides data free to the public. In return, we ask that you follow the PGN data use guidelines. The PGN data are provided by an international group of researchers with a variety of affiliations and institutional support. Each site has a Principal Investigator (PI) and local operators, responsible for deployment, maintenance and data collection. The PI and local operators have invested considerable effort in the production of the data and they are entitled to be informed of any use of data produced by that site.

**Using PGN data**

We suggest consulting with the PI(s) of the instruments about the data to be used, if there are specific questions or apparent issues with the data. While we make an effort to ensure uniformly high data quality, each PGN instrument has a unique location that can affect the representativeness of the data. The PI may have information about the local environment of an instrument that is important in your analysis.

**Publishing PGN data**

*Co-authorship*

We recognize that it is entirely the decision of the primary author of a manuscript to decide upon co-authors. We suggest that if the PGN data from a few sites are a major component of the paper then co-authorship to PI(s) be offered. In the event that co-authorship is not justified, an acknowledgment is sufficient. If PGN data are used in combination with data from other sources and co-authorship is offered to their PIs, then co-authorship should also be offered to the PGN PIs.

**Example acknowledgments**

*Example acknowledgment when using PGN data from a 'few' sites:*

"We thank PI(s) and staff for their effort in establishing and maintaining (site name(s)) sites and (Agency) for funding."

*Example acknowledgment when using data from 'many' sites:*

"We thank the PI(s), support staff and funding for establishing and maintaining the (#) sites of the PGN used in this investigation."

**In all cases to be added to the acknowledgment**

"The PGN is a bilateral project supported with funding from NASA and ESA."

### 5.2.3. The Total Carbon Column Observing Network (TCCON)

The observational data relevant for this project obtained from the Total Carbon Column Observing Network (TCCON) is the dry-air total column CO.

TCCON data are available free of charge but come with a data license and use guidelines. The TCCON data license (https://tccon-wiki.caltech.edu/Main/DataLicense) and data use guidelines https://tccon-wiki.caltech.edu/Main/DataUseGuidelines are reproduced here below.

**TCCON Data License**

*License Terms*

- TCCON data or 'Data' refers to the datasets provided by the individual network partners, which are hosted and accessible at https://tccondata.org
- Downloading and/or using the Data will indicate your acceptance to enter into this license agreement.
- Individual datasets or parts of individual datasets might be licensed under a less restrictive license. If datasets with different licenses are used, the more restrictive license applies.
- This license grants you a perpetual, royalty-free, non-exclusive and non-assignable license to use the Data subject to the terms and restrictions set forth herein.
- You have the right to modify and improve on the Data and said modification or improvement will be proprietary to you.
- In consideration of the royalty-free and collaborative nature of this license agreement, however, you agree to keep the authors informed of the modification and improvement to the Data and hereby grant to TCCON a non-exclusive, unconditional, irrevocable, perpetual and royalty-free right and license to use your modifications or improvements with proper acknowledgement to you as the source.
- All Data are assigned a digital object identifier (DOI). Use of these Data to support a published work must include a citation that includes the Data DOI. The guidelines on proper acknowledgement are described below.
- If the Data is used in a publication, co-authorship may be requested at the discretion of the PIs if the PIs or their co-workers provided substantial intellectual input to the publication and/or if the TCCON data are essential to the analysis (e.g., included in most figures, key results would change without the TCCON data). In this case, the PIs and/or their co-workers will provide comments on the manuscript to the primary authors. A step by step guide on how to procede in this case is attached.
- All other rights, including redistribution, display, and publishing adaptations, are reserved.
- Failure to comply with the terms of this license will result in forfeit of the right to use this data until the issue is resolved to the satisfaction of the appropriate TCCON PIs.

For a Step-by-Step procedure of how to comply with our data license, please see our Data Use Policy Guidelines.

*Attribution / Acknowledgement / Citation*

Acknowledgment: "The TCCON data were obtained from the TCCON Data Archive hosted by CaltechDATA at https://tccondata.org." Other acknowledgments (e.g. for funding of TCCON stations) may be requested.

Please cite the data DOI (example for Ascension):

- Feist, D. G., Arnold, S. G., John, N., & Geibel, M. C. (2014). TCCON data from Ascension Island (SH), Release GGG2014.R0 [Data set]. CaltechDATA. https://doi.org/10.14291/tccon.ggg2014.ascension01.r0/1149285

and at least one of the TCCON overview paper or data version paper:

- Wunch, D., G. C. Toon, J.-F. L. Blavier, R. A. Washenfelder, J. Notholt, B. J. Connor, D. W. T. Griffith, V. Sherlock, and P. O. Wennberg (2011), The Total Carbon Column Observing Network, Philos. Trans. R. Soc. A Math. Phys. Eng. Sci., 369(1943), 2087–2112, doi:10.1098/rsta.2010.0240.
- Wunch, D., G. C. Toon, V. Sherlock, N. M. Deutscher, C. Liu, D. G. Feist, and P. O. Wennberg (2015), The Total Carbon Column Observing Network's GGG2014 Data Version, Pasadena, California, doi:

10.14291/TCCON.GGG2014.DOCUMENTATION.R0/1221662

-- JoshLaughner - 07 Oct 2020

**TCCON Data Use Guidelines**

The TCCON PIs welcome collaboration and encourage the use of our data in all analyses. We ask that users engage with the PIs early in their analysis. This engagement will:

- Help users better understand the limitations of these data and improve the resulting analysis
- Help the network improve our products and our communication of them

Furthermore, citations and publications resulting from this engagement will assist the PIs in their efforts to secure funding to maintain and continue the development of the network.

We encourage you to sign up to the TCCON Users email list to get email updates on TCCON data releases and data use by sending an email with the subject line 'subscribe' to tccon-users-join@caltech.edu.

**Step-by-step procedure**

**When you begin your analysis:**

- Download the public TCCON data and read the associated license for their use.
- You are welcome to share your analyses of the TCCON data with your collaborators. If your collaborators want a copy of the original data files, please direct them to the TCCON archive.
- Contact the relevant PIs if you have questions or concerns. Contact information is included in the metadata associated with each site's dataset.
- You are welcome to sign up for the TCCON users mailing list (send an email with the subject line 'subscribe' to tccon-users-join@caltech.edu), in order to be notified about news and updates.

**When you begin to prepare a formal manuscript or presentation, or plan any commercial use of these data:**

- Download the latest version of the TCCON data and read the associated license for their use.
- Share your analysis of the latest version of the TCCON data with your collaborators. If your collaborators want a copy of the original data files, please direct them to the TCCON archive.
- Contact the relevant PIs. Contact information is included in the metadata associated with each site's data.
    - This contact should occur a minimum of 4-6 weeks prior to the submission of a manuscript and 1-2 weeks prior to a public presentation.
    - If data from many sites are used, you should instead contact the TCCON chair/deputy chair for your region using our online form (https://www.jotform.com/200196634059052) or centralized email address (tccon.ftir@gmail.com). In the email, please include information about which datasets (which TCCON sites) you have used and how important you feel the data were to your study.

**Attribution / Acknowledgement / Citation:**

- Proper attribution and acknowledgment of data in a public presentation will consist of:
    - An acknowledgment of the TCCON science team, and that "The TCCON data were obtained from the TCCON Data Archive hosted by CaltechDATA at https://tccondata.org."
    - Co-authorship may be warranted if the TCCON PIs or their co-workers provided substantial intellectual input to the presentation and/or if TCCON data are essential to the analysis.
- Proper attribution and acknowledgment of data in a publication will consist of:
    - Citation of the DOI for each dataset used and any other relevant publications (a bibtex file for GGG2014 is provided here, and a plain text list of citations is appended to the license linked with the data files; for GGG2020, please use this LaTeX tool to generate a bibliography and table of sites: https://tccondata.org/metadata/siteinfo/genbib/).
    - Citation of the TCCON description paper and/or the data version description paper.
        - Wunch, D., G. C. Toon, J.-F. L. Blavier, R. A. Washenfelder, J. Notholt, B. J. Connor, D. W. T. Griffith, V. Sherlock, and P. O. Wennberg (2011), The Total Carbon Column Observing Network, Philos. Trans. R. Soc. A Math. Phys. Eng. Sci., 369(1943), 2087–2112, doi:10.1098/rsta.2010.0240.
        - Wunch, D., G. C. Toon, V. Sherlock, N. M. Deutscher, C. Liu, D. G. Feist, and P. O. Wennberg (2015), The Total Carbon Column Observing Network's GGG2014 Data Version, Pasadena, California.

- Laughner, J., et al. (in prep), The Total Carbon Column Observing Network GGG2020 Data Version.
- An acknowledgment that: "The TCCON data were obtained from the TCCON Data Archive hosted by CaltechDATA at https://tccondata.org." Other acknowledgments (e.g. for funding of TCCON stations) may be requested.
- At the discretion of the PIs, co-authorship may be requested if the TCCON site PIs, the TCCON algorithm team, or their co-workers provided substantial intellectual input to the publication and/or if the TCCON data are essential to the analysis (e.g., included in most figures, key results would change without the TCCON data). In this case, the PIs will provide comments on the manuscript to the primary authors.

-- JoshLaughner - 07 Oct 2020

### 5.2.4. The Cloudnet network in the ACTRIS Research Infrastructure

The ACTRIS-Cloudnet data portal is at https://cloudnet.fmi.fi/. Data are stored in netCDF, 1 file per station and per day.

Details on the data license are provided on https://docs.cloudnet.fmi.fi/ and are reproduced hereafter.

**License**

Cloudnet data is licensed under a Creative Commons Attribution 4.0 international licence.
This is a human-readable summary of (and not a substitute for) the licence.
You are free to:

- **Share** — copy and redistribute the material in any medium or format
- **Adapt** — remix, transform, and build upon the material for any purpose, even commercially

Under the following terms:

- **Attribution** — You must give appropriate credit, provide a link to the licence, and indicate if changes were made. You may do so in any reasonable manner, but not in any way that suggests the licensor endorses you or your use
- **No additional restrictions** — You may not apply legal terms or technological measures that legally restrict others from doing anything the licence permits

The licensor cannot revoke these freedoms as long as you follow the licence terms.

Citation and acknowledgment information is obtained when clicking on a particular data file link. E..g., for https://cloudnet.fmi.fi/file/1e31e06a-8384-4953-bee2-855082359a1c (Chilbolton data at 25 November 2022) the following information is obtained.

**Citation**

O'Connor, E., and Walden, C. "Classification data from Chilbolton on 25 November 2022", ACTRIS Cloud remote sensing data centre unit (CLU), https://cloudnet.fmi.fi/file/1e31e06a-8384-4953-bee2-855082359a1c, 2022

Please include the following information in your publication. You may edit the text to suit publication standards.

**Data availability**

The data used in this study are generated by the Aerosol, Clouds and Trace Gases Research Infrastructure (ACTRIS) and are available from the ACTRIS Data Centre using the following link: https://cloudnet.fmi.fi/file/1e31e06a-8384-4953-bee2-855082359a1c.

**Acknowledgements**

We acknowledge ACTRIS and Finnish Meteorological Institute for providing the data set which is available for download from https://cloudnet.fmi.fi/.

The data is collected automatically by BIRA-IASB using the metadata harvester from EVDC.

## 5.3. NDACC Zenith-Scattered-Light (ZSL-) UV-visible DOAS data

### 5.3.1. Description

A key property of zenith-sky measurements at twilight is the geometrical enhancement of the optical path in the stratosphere ([RD20:Solomon1987]), which offers high sensitivity to stratospheric absorbers of UV-visible radiation and lower sensitivity to clouds and tropospheric species.

Serving as a reference for the validation of all nadir UV–visible satellites to date since GOME (1995-2011), these measurements are particularly useful for the validation of satellite climate data records and of the stratospheric column subtracted to the total column to obtain the tropospheric column (e.g., the validation of the QA4ECV NO2 ECV precursor data product [RD55:Compernolle2020]). A part of the ZSL-DOAS instruments, the SAOZ network (http://saoz.obs.uvsq.fr/), was used within the project to validate L2 NO2 data [RD8:PVIRv2].

### 5.3.2. Geographical and temporal coverage and sampling

The geographical distribution of NDACC ZSL-DOAS instruments, contributing currently data to the operational validation of S5P TROPOMI $NO_2$, is displayed in Figure 3. Several of these instruments have data records dating back to the nineties, and even the eighties for a few of them (see Figure 4). Where there are different processings of the same data (latmost_v3 or NDACC), differences are small.

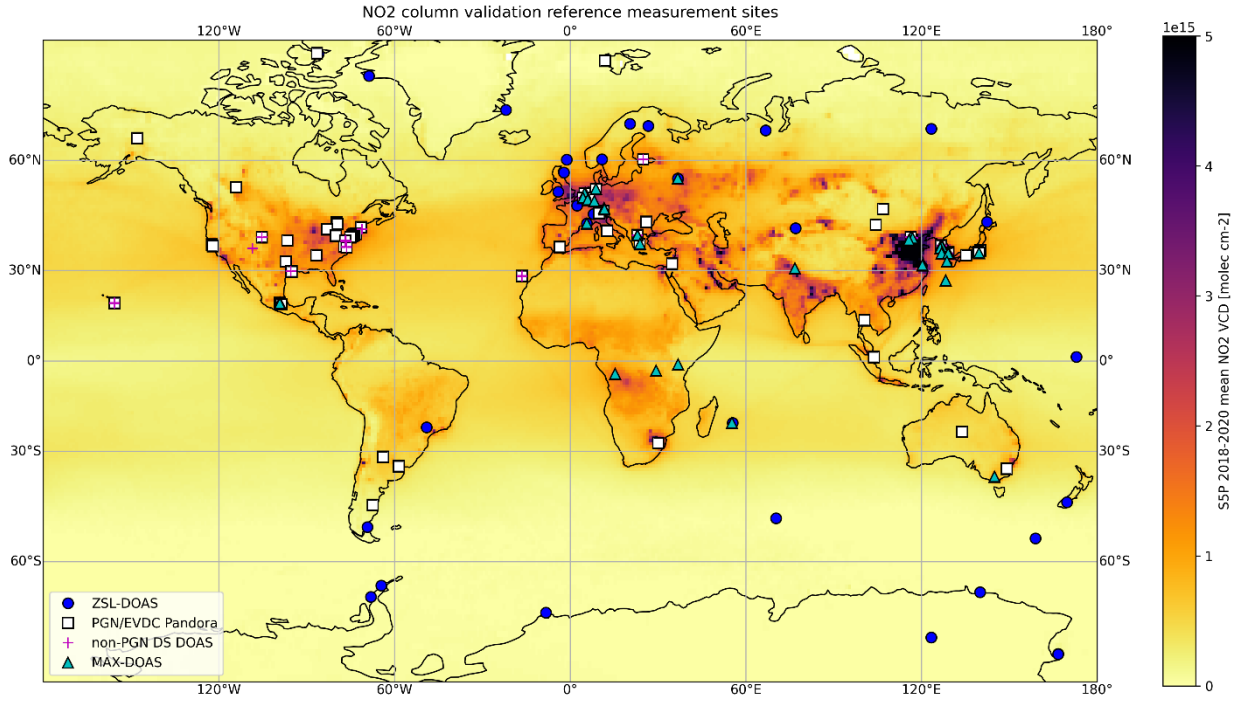



**Figure 3. Geographical distribution of the ground-based UV–Visible DOAS spectrometers planned to contribute NO2 validation reference measurements for the NO2 CDR validation: NDACC ZSL-DOAS (NO2 stratospheric column), NDACC MAX-DOAS (NO2 tropospheric column), PGN Pandora (NO2 total column) and non-PGN direct sun DOAS. The SAOZ part of the ZSL-DOAS data was already used for [RD8:PVIRv2]. Background is a multi-annual mean tropospheric vertical column density (VCD) based on S5P NO2 observations.**

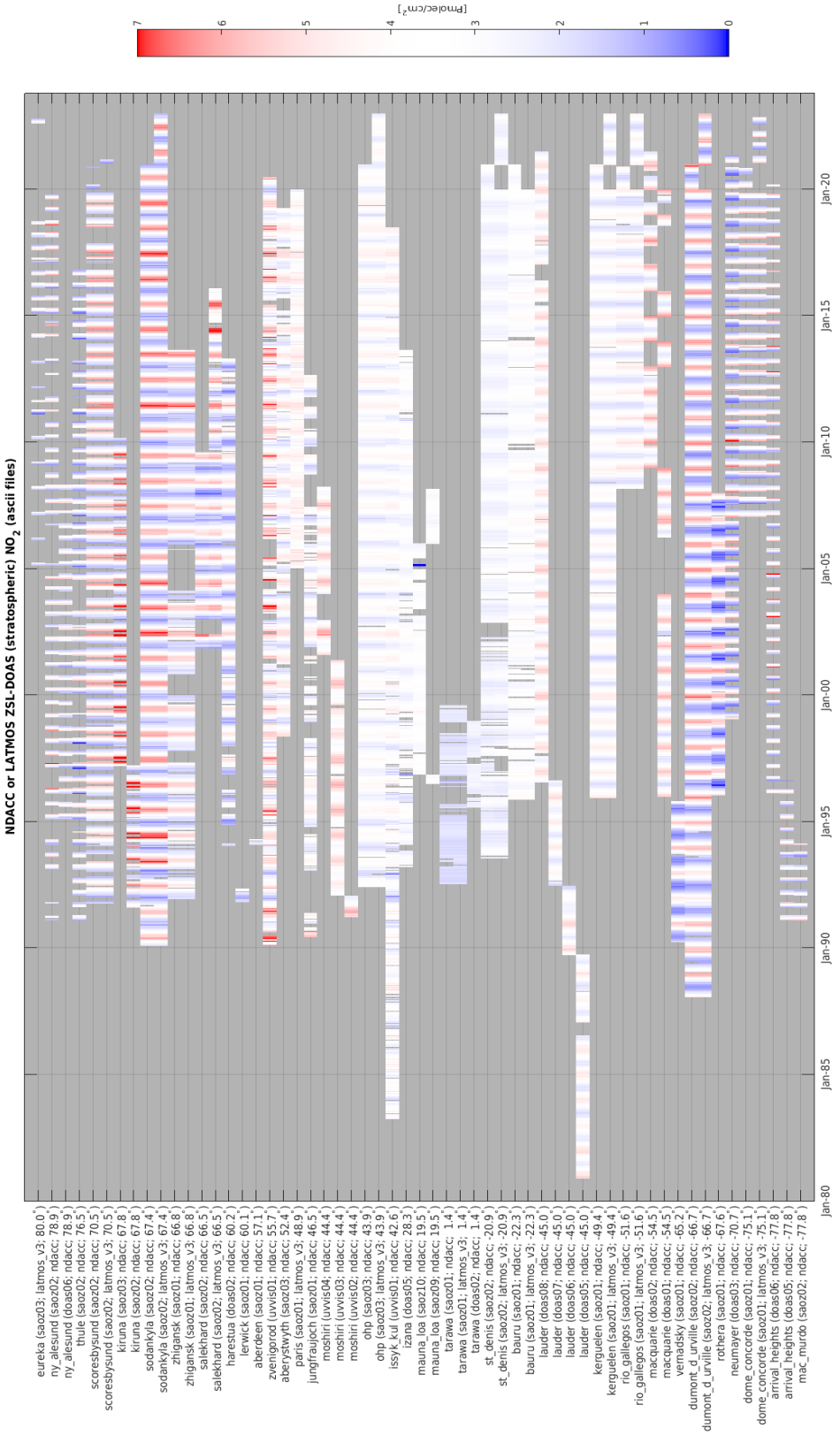



**Figure 4. Temporal distribution of NDACC ZSL-DOAS measurements. Different instrument codes (e.g., uvvis02, uvvis03, …) at the same site imply different instruments. Where there are different processings of the same data (latmost_v3 or NDACC), differences are small.**

### 5.3.3. Data access and data access policy

NDACC ZSL-DOAS data is obtained from the NDACC Data Host Facility (DHF). The data format is NASA AMES ASCII or HDF GEOMS. The NDACC Data Use Agreement is specified in section 5.2.1.

SAOZ ZSL-DOAS data is obtained from http://saoz.obs.uvsq.fr/ and is publicly available. The data is in custom ASCII format.

Both data streams are daily ingested in the Multi-TASTE/CORR-2 validation data base at BIRA-IASB and converted to a format compatible with HARP [RD80:HARP].

### 5.3.4. Uncertainty characteristics

NDACC intercomparison campaigns [RD22:Roscoe1999][RD24:Vandaele2005] conclude an uncertainty of about 4 %-7 % on the $NO_2$ slant column density. After conversion of the slant column into a vertical column using a zenith-sky AMF calculated with assumed vertical profiles of pressure, temperature and UV-visible absorbing species, and for the latest version of the data processing, the uncertainty on the vertical column is estimated to be on the order of 10 %-14 % [RD25:Yela2017][RD21:Bognar2019].

The uncertainty analysis of [RD21:Bognar2019] includes comparisons between different ZSL-DOAS and satellite data. Note that the per-observation uncertainty in the data files does not include all uncertainty sources.

### 5.3.5. Limitations

The geometrical enhancement also implies horizontal smoothing of the measured information over hundreds of kilometres, which requires appropriate co-location methods to avoid large discrepancies with the higher resolution measurements of OMI and TROPOMI.

Furthermore, as these measurements are taken at twilight and stratospheric NO2 has a large diurnal variation, a large temporal co-location mismatch can occur with the satellite measurement. The photochemical adjustment required is introduced in Section 4.1.5.

## 5.4. Multi-Axis (MAX-) UV-visible DOAS data

### 5.4.1. Description

From sunrise to sunset, MAX-DOAS instruments (Honninger et al., 2004 [RD30:Hönninger2004]) measure the UV–visible radiance scattered in several directions and elevation angles, from which the tropospheric vertical column density (VCD) and/or the lowest part of the tropospheric profile (usually up to 3-4 km altitude) can be retrieved with between 1 and 3 degrees of freedom (see, for example, [RD31:Hendrick2014][RD32:Friedrich2019][RD33:Bösch2018][RD34:Irie2011],[RD35:Irie2012]; [RD36:Wagner2011][RD37:Frieß2019]). Their horizontal spatial representativeness varies with the aerosol load and the spectral region of the retrieval, from a few kilometres to tens of kilometres [RD34:Irie2011][RD36:Wagner2011][RD39:Wang2014b].

### 5.4.2. Geographical and temporal coverage and sampling

#### 5.4.2.1. MAX-DOAS $NO_2$ measurements

The geographical distribution of MAX-DOAS instruments measuring **$NO_2$** is provided in Figure 3: data of 38 sites (stations and short-term campaign sites) have been collected from NDACC and from the TROPOMI validation AO project NIDFORVAL, and translated to a common format. The temporal coverage is provided in Figure 5. Note that for some stations, different processings are available. Future harmonization of the data acquisition and processing is expected as a result of the third Cabauw Intercomparison of Nitrogen Dioxide Measuring Instruments (CINDI-3), carried out in May-June 2024.




**Figure 5. Temporal coverage of collected MAX-DOAS NO2 data, covering 43 sites (stations and campaign sites). Note that for some instruments, there are multiple processings; and for some sites multiple instruments. There are 66 datasets in total. Code within brackets refers to the institute. Code explanations: frm01: processed with**

**FRM4DOAS processor; gmap2021, sijaq2022 refer to campaigns; unam_v001-3 refer to different viewing directions. Part of the data is available from NDACC, other data is collected e.g., in the framework of the S5PVT NIDFORVAL project. Stations of Chiba University (aka A-Sky) are marked red: there are restrictions in data policy which likely precludes their use. There are 15 non-ChibaU sites (23 datasets, marked blue) within the GEMS spatial data coverage, but not all contribute within GEMS temporal range (start measurements 2020/11/01, dashed line).**

Currently 15 MAX-DOAS stations (23 datasets) are located within the GEMS measurement area, but not all contribute within GEMS temporal range (start measurements 2020/11/01) and Chiba University stations can likely not be used due to data policy. At the current collection status, 10 (11) datasets contribute in 2021 (2022) respectively, of which 4 (3) over the full year. Much less data is available for 2023 and beyond. From this perspective, it seems best that GEMS NO2 2021 or 2022 is processed, unless considerably more FRM MAX-DOAS data can be collected for the later years.

### 5.4.2.2. MAX-DOAS HCHO measurements

Figure 6 displays the geographical distribution of the MAX-DOAS instruments with **HCHO** data collected for the HCHO CDR validation: 35 sites (stations and campaign sites). While MAX-DOAS data is used for validation from 2005 for NO2 [RD56:Pinardi2020] and from 2007 for HCHO [RD57:DeSmedt2015], most sites start contributing only after 2010-2012.

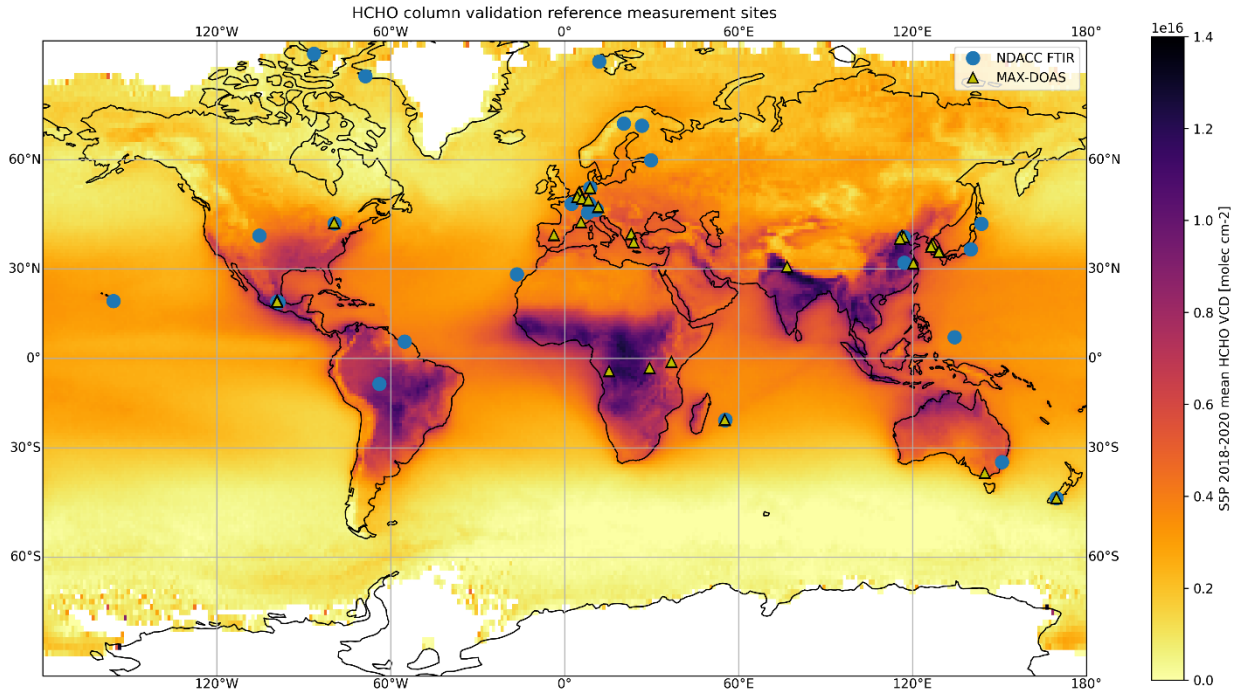



**Figure 6. Geographical distribution of the ground-based UV–Visible MAX-DOAS and FTIR spectrometers that contribute HCHO reference measurements to the CDR validation; all FTIR, and part of the MAX-DOAS, have been used in [RD8:PVIRv2]. Background is a multi-annual mean tropospheric VCD column based on S5P HCHO observations.**

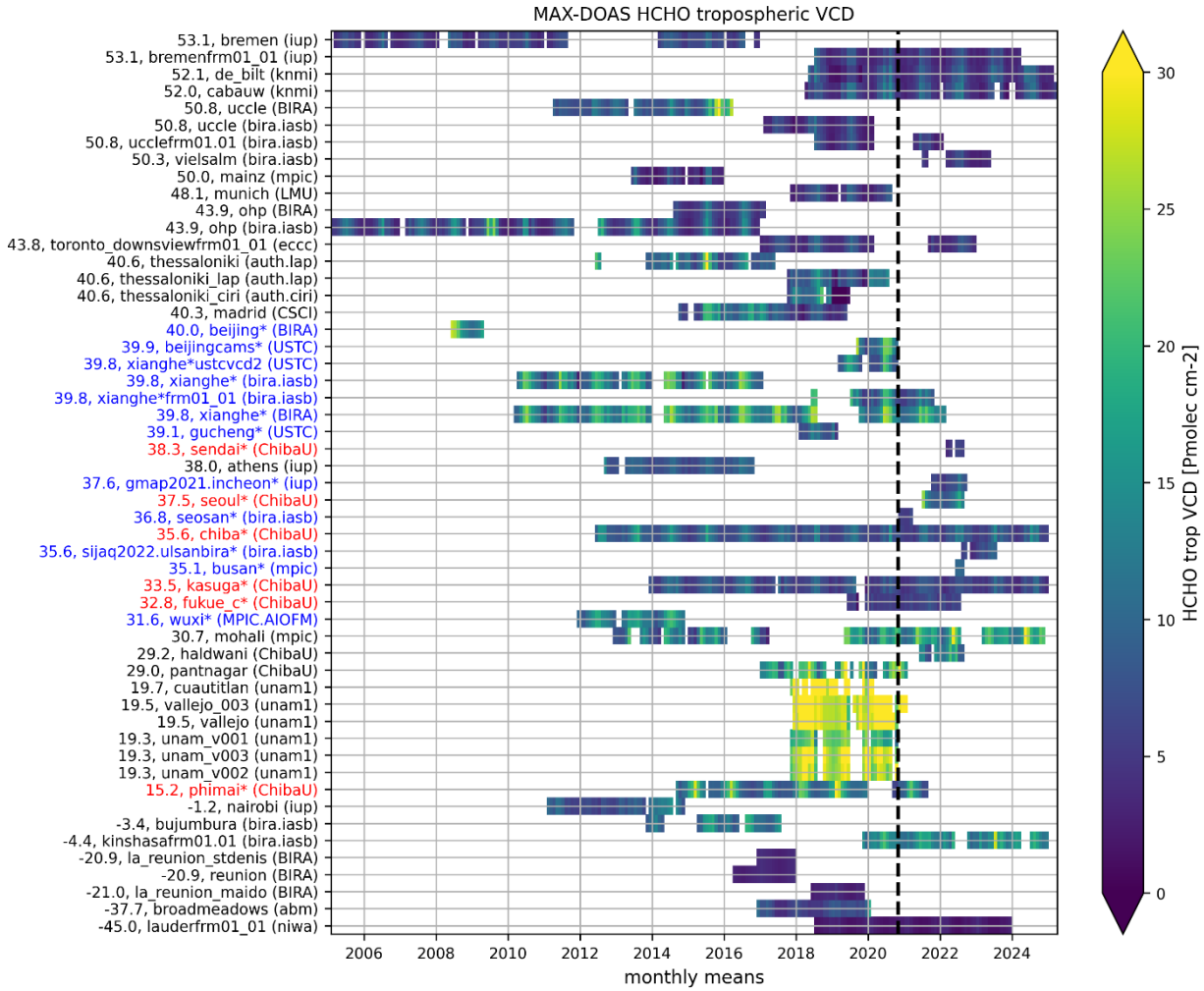



**Figure 7. Temporal coverage of collected MAX-DOAS HCHO data, covering 39 sites (stations and campaign sites). Note that for some instruments, there are multiple processings and for some sites multiple instruments; there are 53 datasets in total. Code within brackets refers to the institute. Code explanations: qa4ecv: QA4ECV processing, with 336-359nm or 324 -359nm window; frm01: processed with FRM4DOAS processor; bepro: bePRO processing; gmap2021, sijaq2022 refer to campaigns; unam_v001-3 refer to different viewing directions at Unam; uccle-sg and uccle-miniDOAS refer to two different instruments at Uccle. Part of the data is available from NDACC, other data is collected e.g., in the framework of the S5PVT NIDFORVAL project. Note that the stations of A-Sky/Chiba University are indicated in red: restrictions in data policy will probably exclude their use. There are 8 non-ChibaU sites (18 datasets, marked blue) within the GEMS spatial data coverage, but not all contribute within GEMS temporal range (start measurements 2020/11/01, dashed line).**

Currently 8 MAX-DOAS stations (18 datasets) are located within the GEMS measurement area, but not all contribute within GEMS temporal range (start measurements 2020/11/01) and Chiba University stations can likely not be used due to data policy. At the current collection status, 6 (5) datasets contribute in 2021 (2022) respectively, of which 1 (0) over the full year. Much less data is available for 2023 and beyond. From this perspective, it seems best that GEMS NO2 2021 or 2022 is processed, unless considerably more FRM MAX-DOAS data can be collected for the later years.

### 5.4.2.3. MAX-DOAS SO2 measurements

For **SO2** the number of MAX-DOAS stations is very limited (Figure 11, Figure 8). The major sources seem to be: (I) routine measurements from BIRA-IASB since 2010 at Xianghe (China), (ii) data for Wuxi (China) covering 2011-2014 shared by the PI [RD61:Wang2017], and translated by us to HARP format, and (iii) MPIC/IISER data from Mohali (India) since 2019, that the PI is willing to share.

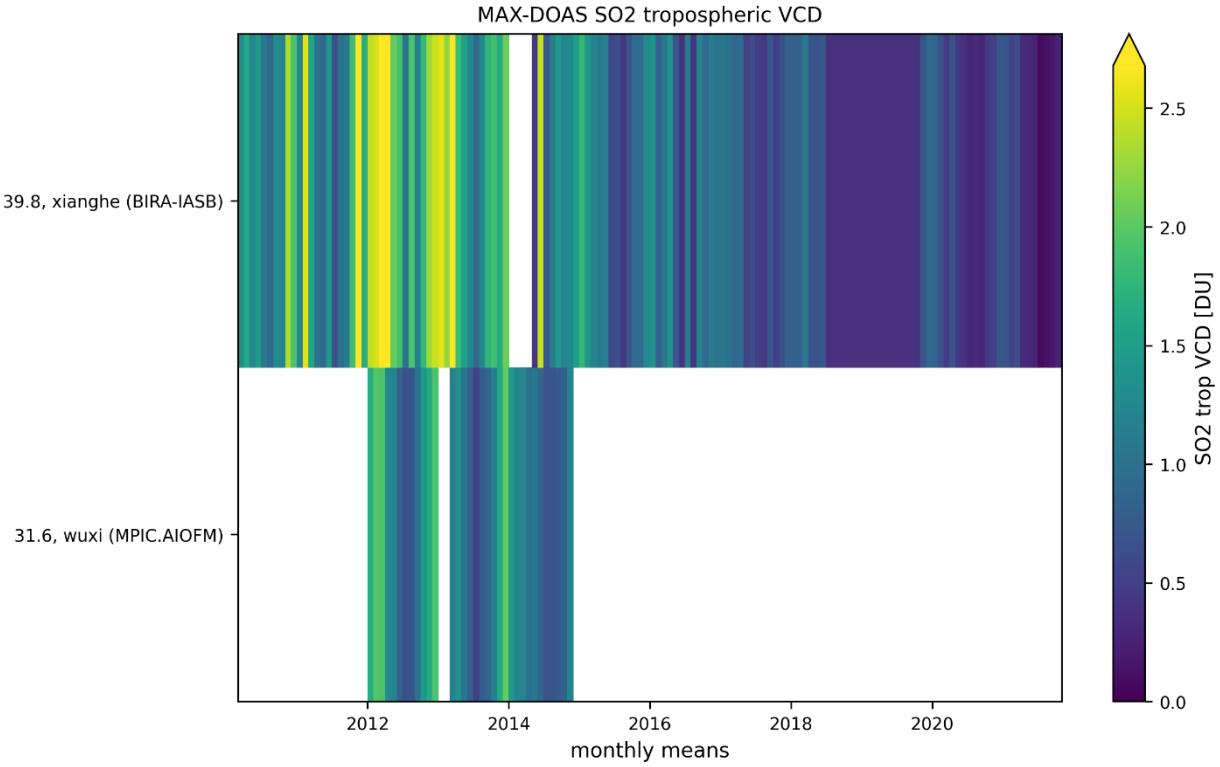



**Figure 8. Temporal coverage of collected MAX-DOAS SO2 data. Code within brackets refers to the institute. Data from Mohali (India) is in principle available but has not been ingested in our system yet.**

### 5.4.2.4. MAX-DOAS CHOCHO measurements

For **CHOCHO**, only the BIRA-IASB or IUP-B stations Uccle (2017-present), Vienna (2018-present), Athens (2018-present), Bremen (2018-present) and Xianghe (2010-present) are currently planned to be used.

### 5.4.3. Data access and data access policy

Data are collected either through EVDC or by direct delivery from the instrument principal investigators, (e.g., within the S5PVT NIDFORVAL AO project). Some of the MAX-DOAS data are part of NDACC. Details about the NDACC use guidelines are provided in section 5.2.1.

Regarding the data in collection directly from the instrument principal investigators:

- NO2 (43 sites, including campaign data) and HCHO data (39 sites, including campaign data) were collected (e.g., in the framework of the S5PVT NIDFORVAL project); only a small subset of these are available at NDACC DHF or EVDC for public use; for the others the use has to be agreed with the data providers. For some sites the data is in HDF GEOMS format (although GEOMS conventions are not always strictly followed) while for others the data is provided in custom ascii format. We should note that there is a data policy regarding the MAX-DOAS NO2 and HCHO data of the A-Sky network (8 Asian stations), resulting in a severe restriction to the data used (Hiroshi Irie, private communication, 2022/12/17). According to the latest update (2024/06), only the use of the Chiba station is endorsed, while for the other sites it is still in consideration. Moreover, the data should be clearly acknowledged as A-SKY/MAX-DOAS data from Hiroshi Irie to differentiate from other MAX-DOAS data. Part of the MAX-DOAS data is centrally processed according to the FRM4DOAS standard and can technically be accessed via EVDC. A significant effort was done in the current project to convert the data to a common format (HARP). Part of the data is already effectively used for HCHO CDR validation in this project [RD8:PVIRv2].
- The MAX-DOAS SO2 data from Xianghe [RD38:Wang2014a] is a research product from BIRA-IASB and available on demand only (private communication, F. Hendrick, BIRA-IASB, 2022/03/09). The data is in HDF GEOMS format. This data has already been used for OMI SO2 validation in this project [RD8:PVIRv2].
- Vinod Kumar and Vinayak Sinha are willing to share the MAX-DOAS SO2 data from Mohali, on condition of accreditation of both MPIC and IISER (private communication, V. Kumar, 2022/03/04). Note the data is in custom text format.
- Yang Wang shared kindly MAX-DOAS data (NO2, HCHO and SO2) for Wuxi (2011-2014) and Xingtai (few months in 2016) (private communication, Y. Wang, 2022/04/20). The data is in custom format. The data has been translated to HARP format by us (2024/06).
- Regarding the validation of CHOCHO, it is planned to use data from IUP-B and BIRA-IASB: Xianghe, Uccle, Athens and Vienna. BIRA-IASB provides the data in HDF GEOMS format and IUP-B in custom ASCII format.

### 5.4.4. Uncertainty characteristics

**NO2.** Published total uncertainty estimates on the NO2 tropospheric VCD are of the order of 7 %–17 % in polluted conditions, including both random (around 3 % to 10 %, depending on the instrument) and systematic (11 % to 14 %) contributions [RD34:Irie2011][RD31:Hendrick2014][RD36:Wagner2011]. But as inhomogeneities between individual instruments exist, expert judgement on the total uncertainty at the network level yields a conservative estimate of 30 % uncertainty in polluted conditions [RD54:Verhoelst2021].

**HCHO.** The estimated total uncertainty on HCHO VCD is of the order of 30 % to 60 % in polluted conditions. This includes both random (∼ 5 % to 30 % depending on instrumental signal-to-noise ratio) and systematic (20 %) slant column contributions [RD41:Pinardi2013].

**SO2**. [RD38:Wang2014a] estimate a total uncertainty on SO2 VCD of 23% (MAX-DOAS in Xianghe), with the leading term (19%) being the uncertainty on the a priori profile. [RD40:Wang2017] estimate a total uncertainty on SO2 VCD of 31% (MAX-DOAS in Wuxi), with the leading term (19%) being the smoothing and noise error.

**CHOCHO**. Due to the preliminary nature of the glyoxal data sets it is difficult to give good uncertainty estimates; it is estimated tentatively at 30-40% (F. Hendrick, BIRA-IASB, private communication 2022/12/01).

### 5.4.5. Limitations

MAX-DOAS observations are sensitive mainly to the lower part of the troposphere, usually up to 3 km of altitude. The spatial field of view is typically much smaller than that of the satellite, which can lead to a large co-location error mismatch for rapidly varying gases such as NO2, SO2, CHOCHO and to a less extent, HCHO.

Historical data record is limited in time for most of the stations and only very few instruments have started operations before the Envisat and OMI era. The retrieval approach has not been harmonized across the network yet. Specifically, for CHOCHO, MAX-DOAS retrievals are quite preliminary.

## 5.5. Direct-Sun UV-visible DOAS data

### 5.5.1. Description

The Pandora instrument infers $NO_2$ and $SO_2$ total column data from direct Sun UV-visible observations. The Pandonia Global Network (PGN) of standardized Pandora instruments acquires data in an automatic way across the globe, at regular frequency throughout the day. The data processing is centralized and uses a standard retrieval. In addition, historical data with older reprocessings of about 15 sites have been obtained directly from the instrument PIs, and direct-sun measurements from MAX-DOAS also contribute

### 5.5.2. Geographical and temporal coverage and sampling

The geographical distribution of Pandora instruments contributing currently to the S5P TROPOMI **$NO_2$** and **$SO_2$** validation is provided in Figure 3 and Figure 11, respectively.

#### 5.5.2.1. Direct-sun DOAS $NO_2$ measurements

Currently 91 PGN/Pandora instruments contribute to the operational validation of S5P TROPOMI $NO_2$ (Figure 3). Their temporal coverage does not extend before 2016, with the exception of Innsbruck and Boulder which started in 2015 and 2014 respectively (Figure 9). The older historical NO2 data cover 17 sites, with earliest data starting in 2008, but most sites contributing after 2012.

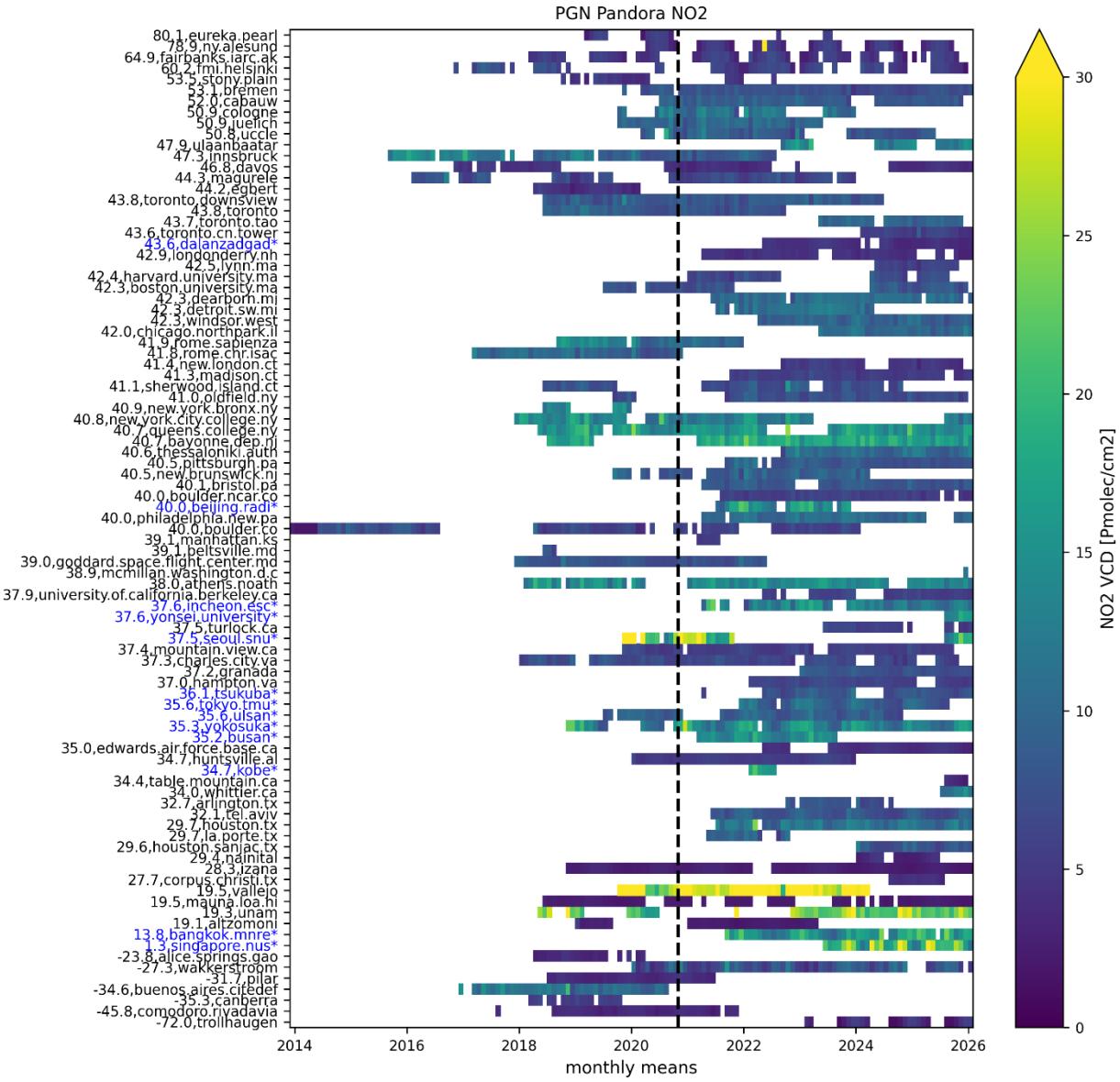



**Figure 9. Temporal coverage of Pandora direct-sun DOAS NO2 VCD measurements from PGN (91 stations), obtained via EVDC. The start of GEMS observations (2020/11/01) is indicated by a dashed line. 13 sites (indicated blue) are within the GEMS spatial coverage.**

*Availability for GEMS NO2 validation:*

Given that only 1 full year of GEMS data will be processed, PGN FRM availability should be checked per year. The best years are 2023, 2022 and 2025, with 10, 10, 9 contributing sites of which 6, 4, 5 have a 12-month coverage. 2021 has the worst availability: considerably less data, and only 1 site with a 12-month coverage.

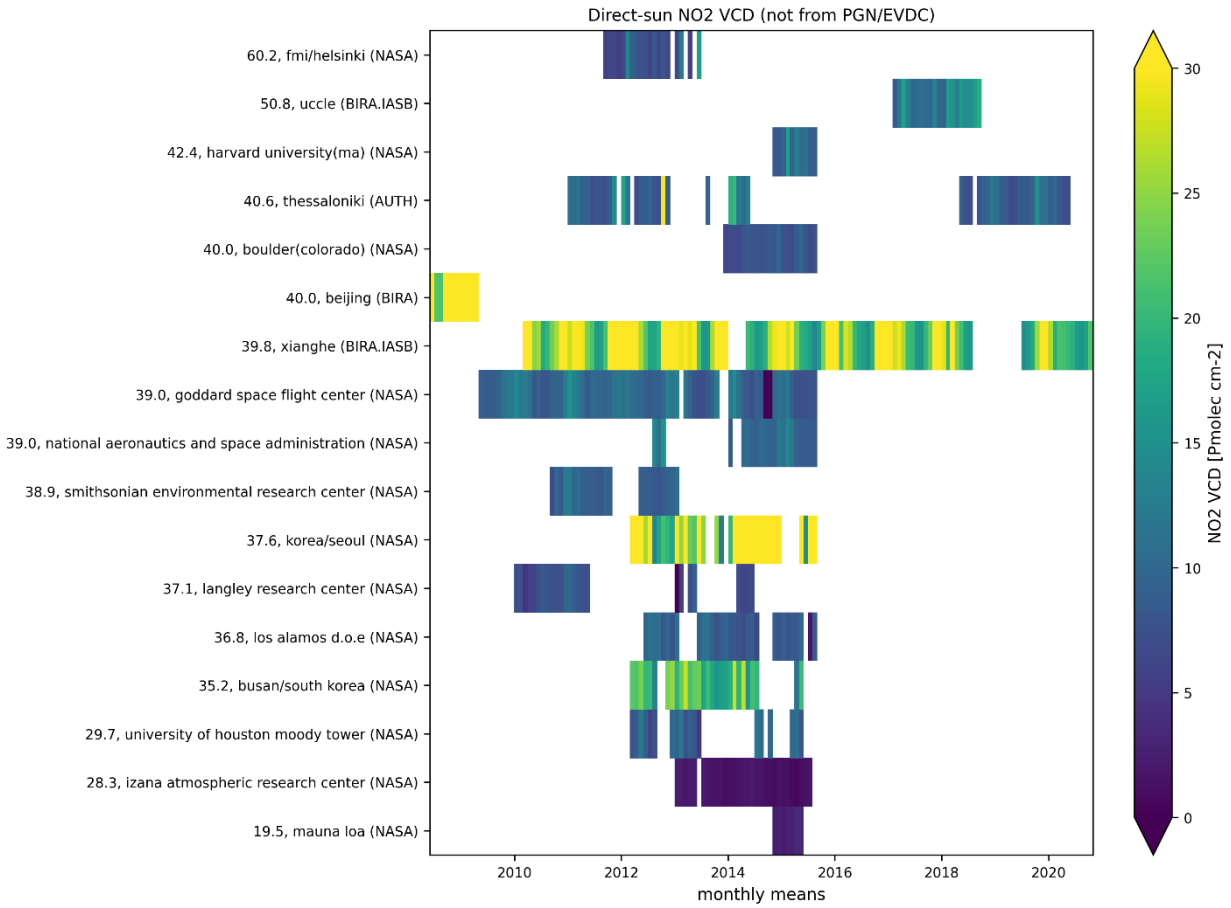



**Figure 10. Temporal coverage of direct-sun NO2 VCD measurements (from Pandora or MAX-DOAS) collected via e.g., the NIDFORVAL project [RD56:Pinardi2020]. Note that this enables access to older data than from PGN.**

### 5.5.2.2. Direct-sun DOAS $SO_2$ measurements

Currently 41 PGN instruments contribute to the operational validation of S5P TROPOMI SO2, with earliest data starting in 2016 (Figure 11, Figure 12) and most only after 2020. But not all locations will be appropriate for satellite validation; only those sites with a clear anthropogenic SO2 signal. The overview in Figure 12 shows that at most measurement sites, values are at noise level. Vallejo, Unam and to a smaller extent Wakkerstroom have a higher SO2 signal, but note that at Vallejo this is partly due to volcanic activity.

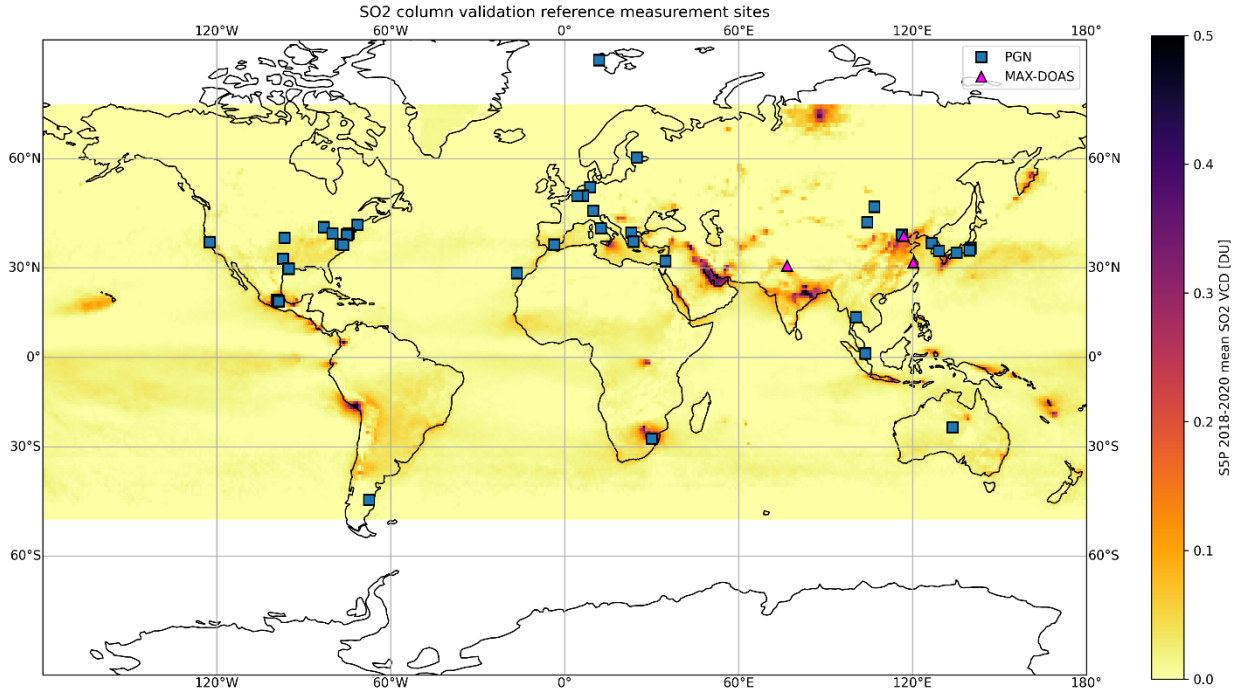



**Figure 11. Geographical distribution of the ground-based UV–Visible spectrometers contributing $SO_2$ reference measurements to the validation of $SO_2$ CDRs: 3 MAX-DOAS and 41 PGN Pandora. The MAX-DOAS at Xianghe is already used in [RD8:PVIRv2]. The background is a multi-annual mean VCD column based on S5P SO2 observations.**

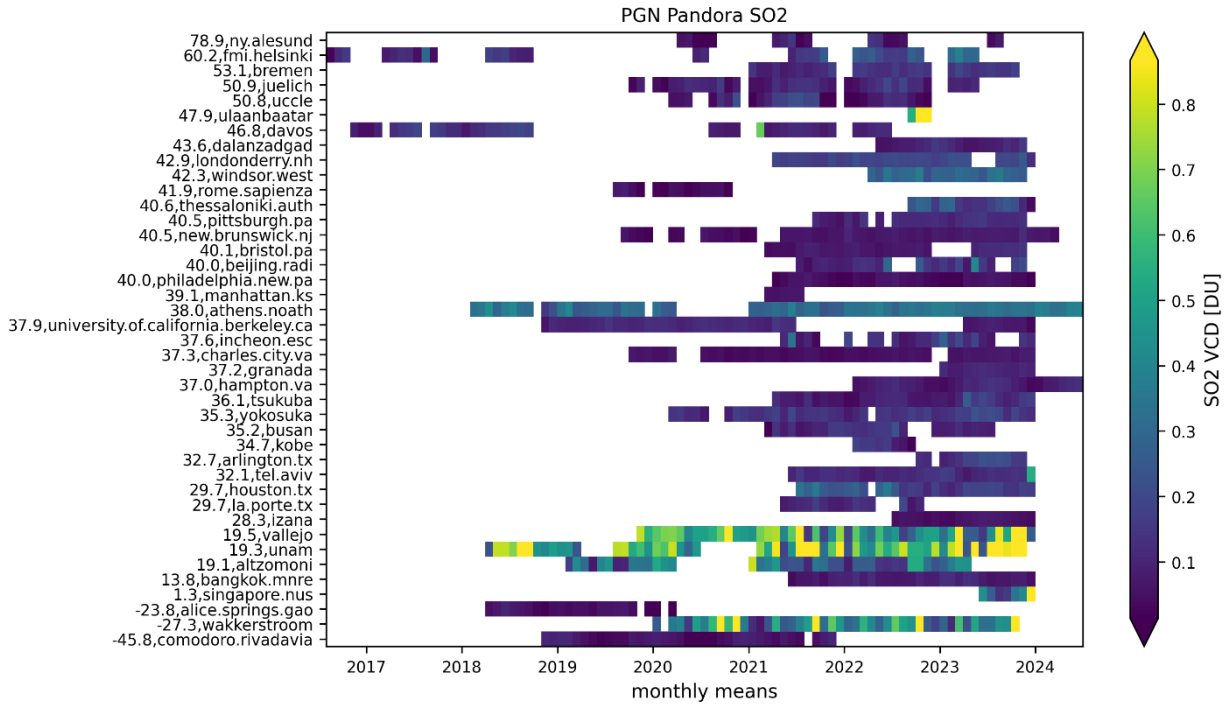



**Figure 12. Temporal coverage of PGN Pandora SO2 measurements (41) stations. Note however the near-zero VCD values at most sites.**

### 5.5.3. Data access and data access policy

Recent data for a large number of sites is available on the Pandonia Global Network data archive. They are uploaded to EVDC while converted to HDF GEOMS format. See section above for more details on the data access and data policy. This data is daily downloaded from EVDC by BIRA-IASB.

The older historical data have been collected from the instrument PIs for 18 sites (a few of them are MAX-DOAS measuring in direct Sun mode). This is non-public data for which use is to be agreed with the PIs. The format is ASCII.

### 5.5.4. Uncertainty characteristics

An uncertainty per measurement is provided. Since the latest PGN data processors rnvs3.1.8 (for NO2) and rsus1.1.8 (for SO2) a distinction is made between 'independent', 'common' and 'structured' uncertainties for data where the error correlation length in time is respectively zero, infinite and non-zero finite. These fields are translated in GEOMS format as 'random uncertainty', 'systematic uncertainty' and 'mixed uncertainty'. PGN data generated with the older NO2 data processor rnvs1p1-7 only reported random uncertainty.

Regarding the NO2 column observations, [RD26:Herman2009] reported a random error uncertainty of about 0.27 Pmolec $cm^{-2}$ and a systematic error uncertainty of 2.7 Pmolec $cm^{-2}$ . However, the newer PGN NO2 rnvs3.1.8 data have considerably lower uncertainties, with a per-site median value of 0.34 Pmolec $cm^{-2}$. This is due to changes in (1) the optical setup, (2) the gas-calibration approach and (3) a more accurate NO2 effective temperature estimation (M. Tiefengraber, private communication [RD29:Tiefengraber2017]).

Regarding the SO2 column observations, [RD27:Fioletov2016] reports a random error uncertainty of about 0.17 DU (4.6 Pmolec $cm^{-2}$ ) and a total uncertainty below 0.3 DU (8 Pmolec $cm^{-2}$) for the Pandora at Fort McKay. The uncertainty reported in the PGN data files is considerably lower, with a per-site median value of 0.035 DU (0.9 Pmolec $cm^{-2}$). As for PGN NO2, this is due to changes in (1) the optical setup and (2) the gas-calibration approach. A third improvement for SO2 is the consideration of the significant cross-correlation between O3 effective temperature and SO2 [RD29:Tiefengraber2017].

Finally, we note that Luftblick and the community have considered all uncertainty sources known to them, and think no major uncertainty sources are missing from the budget [RD29:Tiefengraber2017]. More information about the uncertainty characterisation and validation of PGN data can be found in [RD28:FRM4AQ].

### 5.5.5. Limitations

Only column data is available at EVDC, no profile information. Application of the satellite vertical averaging kernel is therefore not possible. The spatial field of view is typically much smaller than that of the satellite, which can lead to a large comparison error for rapidly varying gases such as NO2 and SO2. For most stations, time series do not extend before 2018.

### 5.5.6. Maturity as a Fiducial Reference Measurement

The maturity as Fiducial Reference Measurement (see section 5.1.1) is determined in Table 17. This applies to the Pandora data (v1.8) from PGN only, not to historical Pandora data.

**Table 17. Maturity as Fiducial Reference Measurement determined for Pandora PGN v1.8 data.**

| FRM CHARACTERISTIC | FULFILLED (YES/NO/PARTIALLY) | REMARK |
|---|---|---|
| Traceability to community-accepted standards and best practices | Yes | Details on the calculation available at https://www.pandonia-global-network.org/home/documents/reports/ |
| Independent from satellite measurement | Yes | Different sensors, processing algorithm |
| Uncertainty budget | Yes | Uncertainty split in independent, common and structured contributions |
| Community-accepted best practices<br>• measurement protocol<br>• processing<br>• archiving<br>• documentation<br>Defined, published openly, adhered to | Yes | See https://www.pandonia-global-network.org/home/documents/reports/ |
| Easily accessible | Yes | Data available at EVDC |
| Fully characterized and regularly calibrated | Yes | See https://www.pandonia-global-network.org/home/documents/reports/ |
| State-of-the-art processing codes | Yes | See https://www.pandonia-global-network.org/home/documents/reports/ |
| Quality indicator traceable to reference standards | Yes | Data quality flag variable<br>Uncertainty variable |

### 5.5.7. Maturity of Data Uncertainty estimates

The maturity of the Data Uncertainty estimates (see section 5.1.2) is determined in Table 18. This only applies to the Pandora data (v1.8) from PGN, not to the historical Pandora data. 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).

**Table 18. Maturity of Data Uncertainty estimates determined for Pandora PGN v1.8 data.**

| 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 |

## 5.6. Fourier Transform Infra-Red spectrometer data

### 5.6.1. Description

The FTIR instruments take absorption measurements of solar radiation under clear-sky conditions, in the mid-infrared for NDACC affiliated instruments and in the shortwave infrared for TCCON affiliated instruments. Many of the NDACC FTIR stations were already active at the beginning of IASI operation in 2007, which allow the validation of the satellite climate data records in the long term and under an extensive variety of atmospheric conditions.

**HCHO**. The FTIR network that has recently adopted a harmonized HCHO retrieval strategy [RD42:Vigouroux2018], and which has been used for S5P HCHO validation (Vigouroux et al., 2020) [RD59:Vigouroux2020]. Currently 29 FTIR stations provide HCHO data. Some of these stations, affiliated to NDACC, started their measurements in the mid 90's and will be particularly useful for the validation of the long-term (merged) CDRs. The degree of freedom of the signal for the profile retrieval is low, about 1.1. The FTIR total column averaging kernel shows a decrease in sensitivity near the surface, quite similar to, e.g., TROPOMI sensitivity.

**CO**. Two ground-based networks of Bruker high-resolution spectrometers were considered for the CO reference data for CDR validation: (i) NDACC FTIR (mid-infrared), providing CO vertical profiles (about 3 Degree of Freedom of the Signal) in addition to total columns, and (ii) TCCON (shortwave infrared) [RD43:Wunch2011][RD44:Wunch2015], providing column-averaged dry-air mole fractions (XCO) and a total column Averaging Kernel. The NDACC FTIR has already been used for validation within the current project [RD8:PVIRv2]. Regarding the TCCON data, it was found that the prior needs to be updated before the data can be used.

**NH3**. Currently, 15 FTIR stations provide $NH_3$ data (Dammers, E. and Van Damme, M., private communication) [RD45:Dammers2015] that can be used for the IASI validation, covering regions with very low to very high $NH_3$ concentrations, which is ideal to assess if the satellite can measure in all conditions with the same precision and accuracy. Currently, 3 high-altitude stations (Maido, Jungfraujoch, Zugspitze) had to be excluded since for $NH_3$ validation (as opposed to HCHO or CO validation) not sufficient information is available for the altitude correction, leaving 12 stations to use for validation.

### 5.6.2. Geographical and temporal coverage and sampling

#### 5.6.2.1. FTIR HCHO measurements

29 FTIR instruments contribute data to the HCHO CDR validation. Their geographical distribution is provided in Figure 6 and the temporal coverage in Figure 13. Six of these sites (Ny-Ålesund, Kiruna, Zugspitze, Rikubetsu, Mauna Loa, Wollongong) provided data since the mid-nineties [RD42:Vigouroux2018].

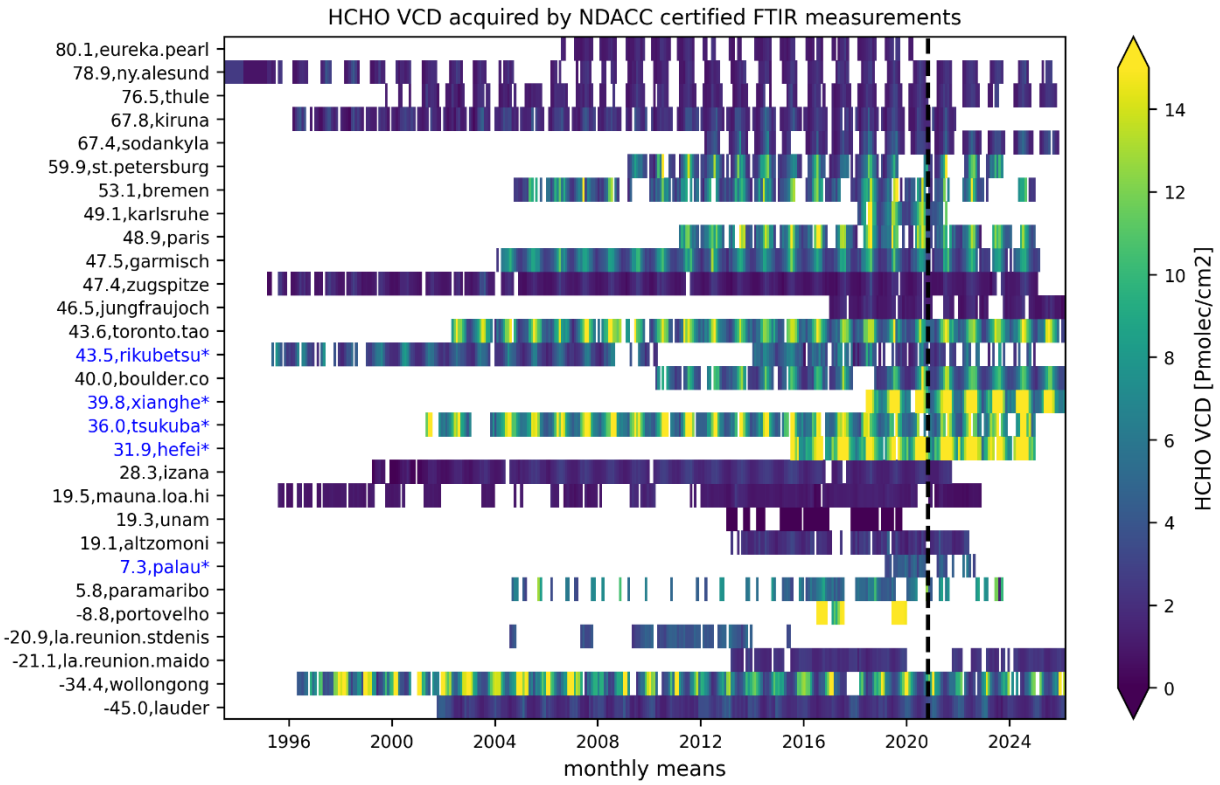



**Figure 13. Temporal coverage of HCHO VCD measurements from 29 stations,by NDACC certified FTIR measurements, used for the HCHO CDR validation. 5 stations are located spatially within GEMS coverage (indicated in blue). GEMS observations start in 2020/11/01 (dashed line).**

*Availability for GEMS HCHO validation:*

5 stations are located within GEMS spatial coverage. Given that only 1 full year of GEMS data will be processed, FTIR FRM availability should be checked per year. 5 sites contribute in 2021 and 2022, 2 of which with a 12-month coverage (Hefei and Xianghe). 4 sites contribute in 2023 and 2024 (Palau then does not contribute), with Xianghe and Hefei having 11 or 12-month coverage.

### 5.6.2.2. FTIR CO measurements

Figure 14 provides an overview of the geographical distribution of the NDACC FTIR instruments that contribute reference data to CO CDR validation. Many of the ground-based stations were already active in 2007, which allows for the validation of the long term (merged) IASI satellite time-series.

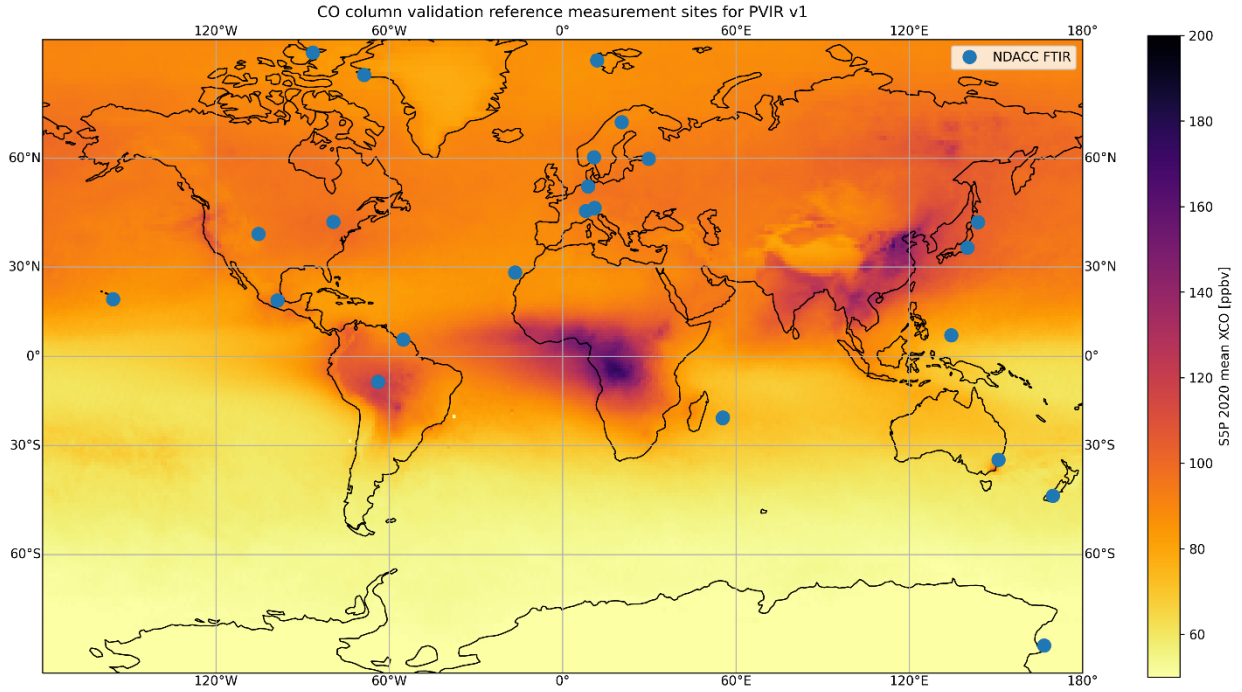



**Figure 14. Geographical distribution of the ground-based NDACC FTIR spectrometers that contribute CO validation reference measurements and used in [RD8:PVIRv2]. Background is a 2020 mean CO column based on S5P CO observations.**

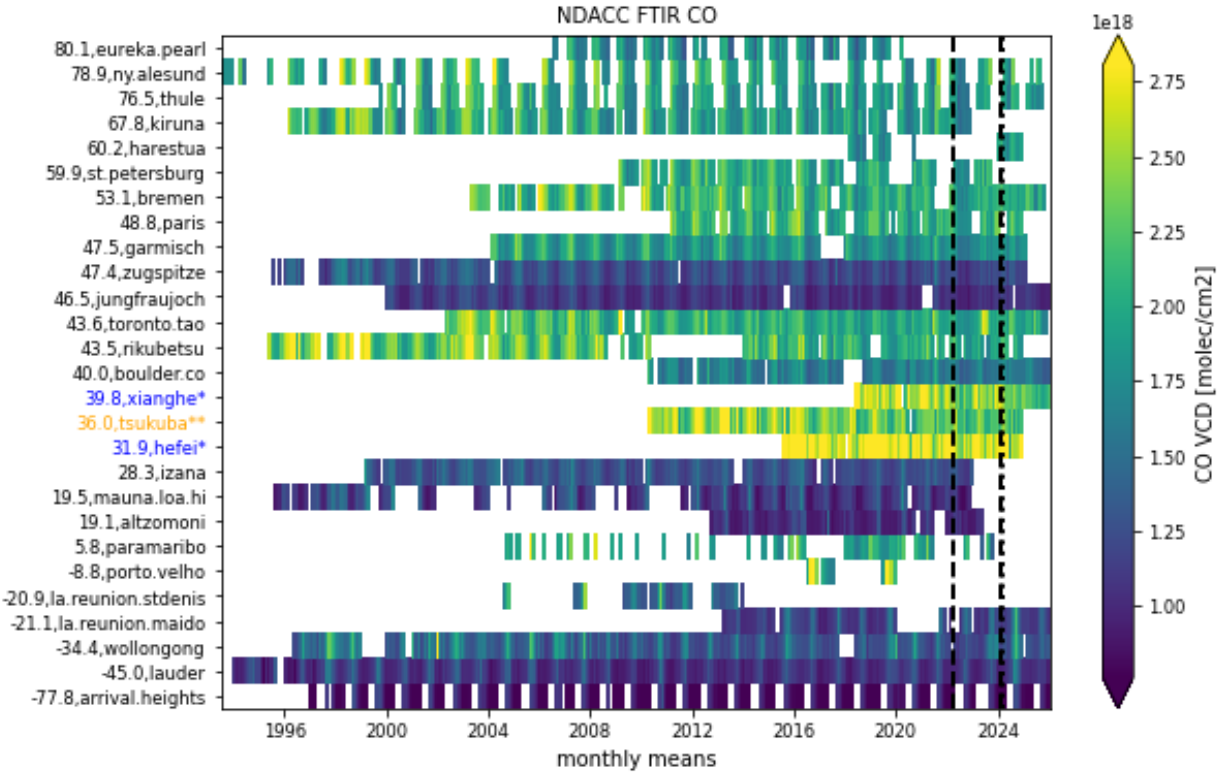



**Figure 15. Temporal coverage of NDACC FTIR CO VCD measurements from 27 stations. Dashed, dotted lines indicate start of GIIRS-B (2022/04/12), end of nominal operations before relocation (2024/01/31) and start again**

**of nominal operations after relocation (2024/02/27). Two sites, Xianghe and Hefei are well within GIIRS spatial coverage, while Tsukuba is an edge case, especially after the GIIRS-B relocation.**

*Availability for GIIRS-B validation:*
Given that only 1 full year of GIIRS data will be processed, FTIR FRM availability should be checked per year. 2 stations (Hefei, Xianghe) are located well within GIIRS-B spatial data coverage, while Tsukuba is an edge case, especially after the GIIRS relocation in 2024/02. All 3 stations contribute in 2023 and 2024. From FRM availability perspective, it is advisable to process 2023, before the GIIRS relocation.

### 5.6.2.3. FTIR $NH_3$ measurements

Figure 16 provides the geographical distribution of the FTIR instruments contributing reference data to the $NH_3$ validation.Note that the FTIR instruments are NDACC certified, but the NH3 column measurements are not an NDACC product. Nonetheless, for some stations the data is pushed to NDACC. As for HCHO and CO validation, many of the NDACC FTIR stations were already active in 2007, which will allow for the validation of the long term (merged) IASI satellite time-series.

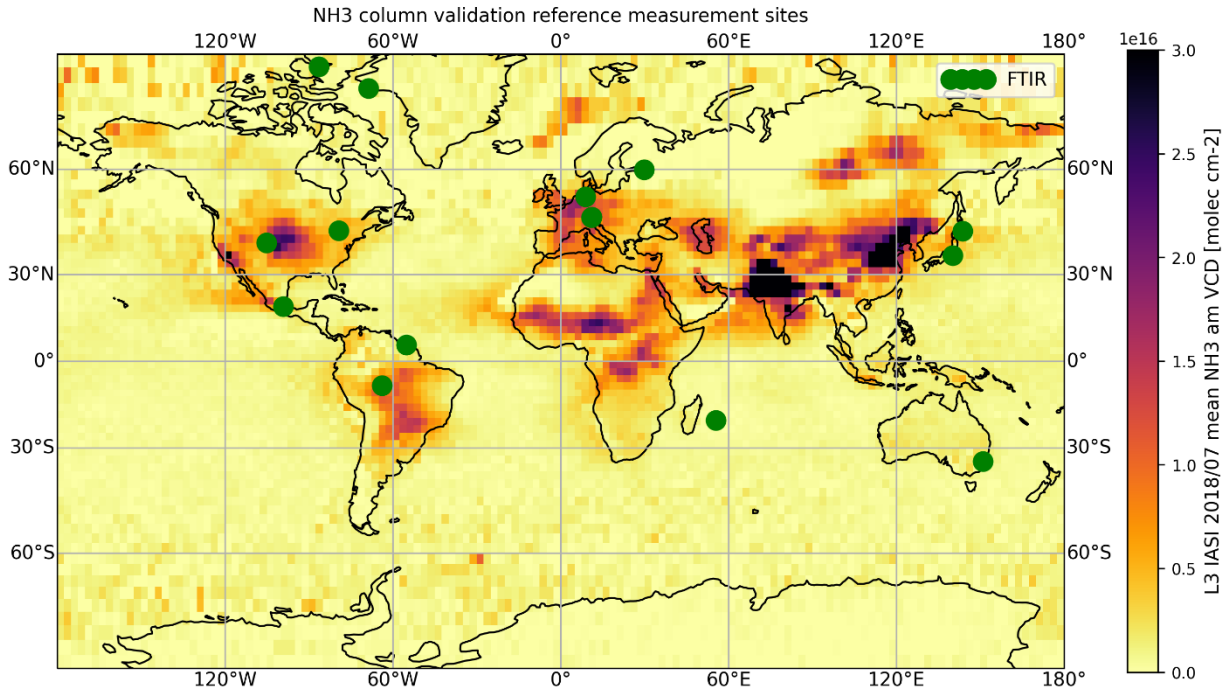



**Figure 16. Geographical distribution of the ground-based FTIR spectrometers contributing NH3 validation reference measurements.**

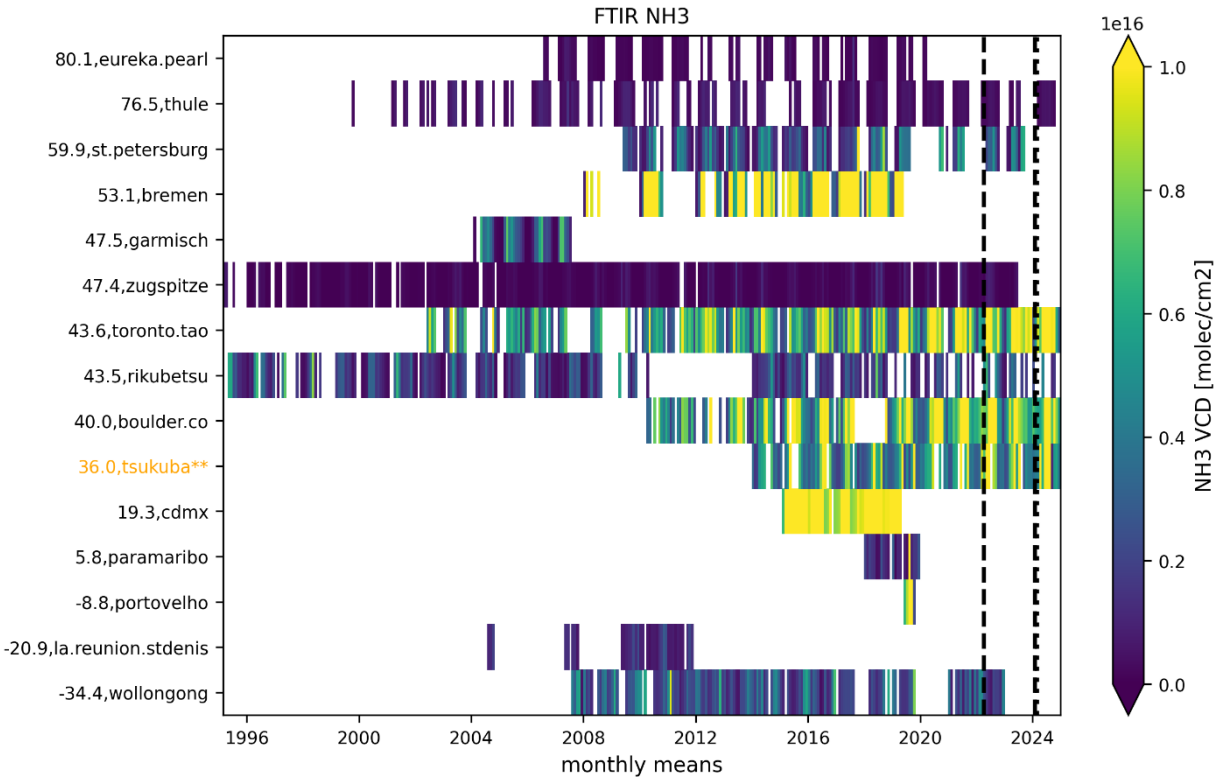



**Figure 17. Temporal coverage of FTIR $NH_3$ measurements from 15 stations. Note that there are 3 high-altitude stations (Ny Alesund, Jungfraujoch, Maido), for which prior profile data is needed to do an altitude correction. Note that Hefei (not present yet in this figure), $NH_3$ data can be obtained from the PI. The dashed lines indicated the start of GIIRS-B measurements and the re-location of GIIRS-B.**

*Availability for GIIRS-B validation:*

Regarding the GIIRS-B validation, currently only the FTIR Hefei is well within GIIRS-B spatial coverage, while Tsukuba is an edge case, especially after the GIIRS-B relocation (2024/02). Note that for FTIR $NH_3$, data can only be obtained on request: for both Hefei and Tsukuba this is still to be done to match GIIRS-B temporal range. The FTIR at Xianghe does not measure $NH_3$. From FRM availability perspective, it seems advisable to process 2023, before the GIIRS-B relocation.

### 5.6.3. Data access and data access policy

The data policy for NDACC FTIR is detailed in section 5.2.1 and for TCCON CO in section 5.2.3.

**NDACC FTIR CO** data is obtained from the NDACC DHF and is available in GEOMS HDF format. Around 20-25 sites are expected to contribute to this study.

**TCCON CO** data [RD43:Wunch2011][RD44:Wunch2015]is publicly available from https://tccondata.org/ in netCDF format; it is also available at EVDC, in HDF format following GEOMS conventions. Depending on the exact version to be used (GGG2020 or GGG2014) we expect 20-28 contributing sites. Note that some sites contribute both to TCCON and NDACC.

**FTIR HCHO** data was collected in the framework of the S5PVT project NIDFORVAL. For part of the sites the data is available at NDACC DHF and EVDC. The number of sites is expected to grow as HCHO has recently become an official NDACC species and more PIs will contribute to NDACC. But not all NIDFORVAL sites will contribute to NDACC in short term as they are not NDACC-affiliated. Data not yet on NDACC should be considered not public. Data format is GEOMS HDF.

The **NH3 FTIR** time series is not public. It was directly obtained from the PIs via Enrico Dammers [RD45:Dammers2015] and used for the validation of IASI [RD64:Dammers2016]. The data format is GEOMS HDF.

### 5.6.4. Uncertainty characteristics

**HCHO**. The FTIR uncertainty budget is calculated following the formalism of [RD75:Rodgers2000] and is described in [RD42:Vigouroux2018]. It is separated into random and systematic components. The random uncertainty is dominated at all sites by the measurement noise uncertainty, which can vary from site to site depending on the spectrometer. The smoothing uncertainty in the total column has a non-negligible random component. Median network values for the random uncertainties are 2.9 $10^{14}$ molec $cm^{-2}$ and 2.3 $10^{14}$ molec $cm^{-2}$ when including or not including the smoothing error. Median network values for systematic uncertainty is 13%, which is dominated by spectroscopic parameters.

**CO**. The typical systematic and random uncertainty of the NDACC FTIR CO data are about 3 % and 1 %, respectively (Sha et al., 2021 [RD62:Sha2021]). The TCCON XCO systematic uncertainty is estimated to 2%, and the random uncertainty is below 4 % and decreases with SZA (Wunch et al., 2015 [RD44:Wunch2015]).

**NH3**. The random uncertainty of a single FTIR NH3 total column measurement is estimated to 9% (polluted site) up to 25% (very clean site), and the systematic uncertainty is about 20-27% and dominated by the uncertainty on the spectroscopic parameters (Dammers et al., 2015 [RD45:Dammers2015]).

#### 5.6.5. Limitations

General. As these are direct Sun measurements, they are limited to clear-sky conditions. The spatial field of view is typically much smaller than that of the satellite, which can lead to a large comparison error for rapidly varying gases such as HCHO and $NH_3$.

HCHO. The degrees of freedom for signal of the profile retrievals is low, about 1.1, meaning there is essentially one piece of information.

## 5.7. Cloudnet radar/lidar data

### 5.7.1. Description

A European network of vertically pointing cloud radars and lidars/ceilometers use the Cloudnet processing scheme [RD46:Illingworth2007] for the continuous evaluation of cloud profile properties. This network is a major contributor to the European Research Infrastructure Aerosol, Clouds and Trace Gas Infrastructure Network (ACTRIS). The Cloudnet scheme combines the cloud radar and lidar measurements at a temporal resolution of 30 s and a vertical resolution of 30 m to create a target categorization product which diagnoses the presence or absence in each altitude bin of aerosol, insects, drizzle, rain, liquid cloud droplets, supercooled liquid droplets, ice cloud particles, and melting ice cloud particles. Note that multiple targets can be diagnosed within a single altitude bin. The Cloudnet L2 classification product then takes the target categorization product and simplifies the possible combinations into 11 main atmospheric target classifications at the same resolution (30 s and 30 m). From the classifications a cloud base height and cloud-top height are also derived and stored in the product. For the validation of satellite-observed cloud heights, we will make use of the cloud top height provided directly in the data file, and also construct an effective cloud middle height from the cloudy altitude bins in the vertical cloud profile [RD66:Compernolle2021].

Cloudnet data have been adapted to and used as a reference data during the round-robin evaluation of the Precursors_cci+ project, for comparisons with the satellite cloud products S5P OCRA\ROCINN and S5P FRESCO-S which are themselves input to S5P $NO_2$, HCHO and $SO_2$. They can be re-used in future Precursors_cci+ related work.

### 5.7.2. Data access and data access policy

Data access and policy are described in Section 5.2.4.

### 5.7.3. Geographical and temporal coverage and sampling

The geographical distribution of Cloudnet instruments, as used for S5P MPC cloud product validation, is provided in Figure 18. Currently 28 stations contribute. Coverage is much reduced when going back in time, i.e., only 4 sites contributed in 2010.

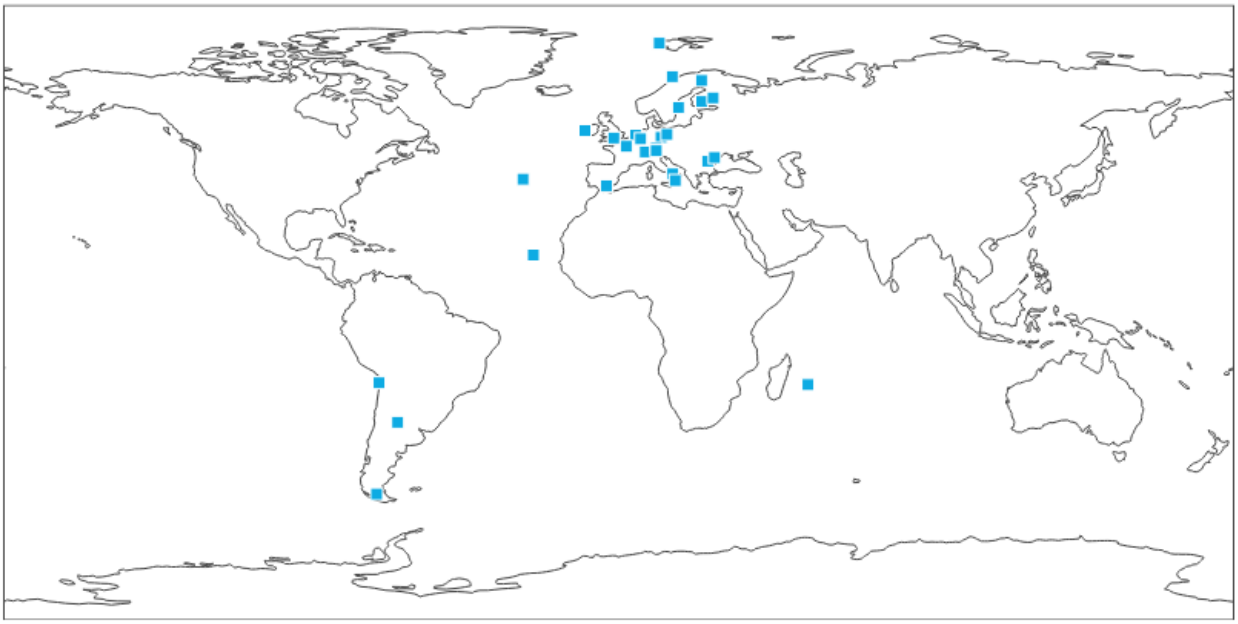


**Figure 18. Geographical distribution of the Cloudnet stations contributing to the operational validation of S5P TROPOMI cloud data products.**

### 5.7.4. Uncertainty characteristics

The variables of use (cloud top height, cloud base height, altitude bin classifications) are not provided with an uncertainty per measurement.

### 5.7.5. Limitations

The sensitivity of the satellite observations to clouds differs significantly from the sensitivity of CLOUDNET/ARM lidar/radar instruments used as a reference. For most of the stations the data do not extend back far in time.

# 6. Compliance with Document Requirement Definitions

This section reviews the compliance of this PVP with the Document Requirement Definitions provided on Page 6 of CCI+ Phase 2 Theme (I) – Precursors ECV SoW – Annex A - [RD4:DRD].

**Table 19. Mapping between SoW *Document Requirements Definitions* for the Precursors_cci+ PVP (Annex A, Page 6) and this Version 1 of the *Product Validation Plan*.**

| SOW ANNEX A REQUIREMENT: THE PVP SHALL … | LINK TO SECTION | REMARKS |
|---|---|---|
| define the design of the validation activity and the methods used to validate the products and their associated uncertainty estimates. | 4 | |
| describe any tools or matchup databases to be used | 4.1.5 | |
| list all reference data sets used to validate each ECV | 5, Table 14, mosaic plots in section 5. | |
| describe the uncertainty characteristics of all reference data | 5.3.4 (ZSL-DOAS), 5.4.4 (MAX-DOAS), 5.5.4 (PGN), 5.6.4 (FTIR), **5.7.4** (Cloudnet) | |
| describe any limitations in the reference data, such as limited sampling (e.g. clear sky only, daytime only) or mismatches with the satellite measurement conditions, or differences between the reference measurement and the satellite-observed quantity (e.g. skin vs. bulk temperature) | 5.3.5 (ZSL-DOAS), 5.4.5 (MAX-DOAS), 5.5.5 (PGN), 5.6.5 (FTIR), **5.7.5** (Cloudnet) | |
| specify how the validation data were accessed and whether these are open and publicly available or whether these data are protected. If the latter is the case, the data access policy shall be included. | 5.2.1 (NDACC), 5.2.2 (PGN), 5.2.3 (TCCON), 5.2.4 (Cloudnet) | |
| identify any community validation protocols or standards to be followed | 4.1 (generic validation protocol and practices), 4.2 (community specifics), 7 (terms and definitions) | |
| define the validation metrics to be used (RMSD, bias, confusion matrices, user/producer accuracies, kappa coefficient, etc.) | 4.1.4 | |
| list all satellite and model data sets to be used for intercomparison | 4.1.8 | Possibilities for satellite intercomparisons are limited. |
| discuss any mismatches between the ECV products and the data sets used for intercomparison (e.g. different observing times, different resolutions, etc.) | 5.3.5 (ZSL-DOAS), 5.4.5 (MAX-DOAS), 5.5.5 (PGN), 5.6.5 (FTIR), **5.7.5** (Cloudnet) | |

# 7. Terms, abbreviations and definitions

## 7.1. Terms and definitions

In Table 20 terms and definitions as recommended by the CEOS WGCV and by standardization bodies have been reproduced.

**Table 20. Recommended terms and definitions.**

| TERM | DEFINITION | SOURCE |
|---|---|---|
| accuracy | closeness of agreement between a quantity value obtained by measurement and the true value of the measurand; note that it is not a quantity and it is not given a numerical quantity value | VIM, GUM |
| area (volume) of representativeness | the area (volume) in which the concentration does not differ from the concentration at the station by more than a specific range | Larssen |
| bias | (1) systematic error of indication of a measuring system<br>(2) estimate of a systematic measurement error<br>(3) estimate of a systematic forecast error | VIM<br>VIM<br>GAS |
| calibration | (1) the process of quantitatively defining the system responses to known, controlled signal inputs<br>(2) operation that, under specified conditions, in a first step, establishes a relation between the quantity values with measurement uncertainties provided by measurement standards and corresponding indications with associated measurement uncertainties and, in a second step, uses this information to establish a relation for obtaining a measurement result from an indication | CEOS<br>VIM |
| dead band (or neutral zone) | maximum interval through which a value of a quantity being measured can be changed in both directions without producing a detectable change in the corresponding indication | VIM |
| detection limit | measured quantity value, obtained by a given measurement procedure, for which the probability of falsely claiming the absence of a component, given a probability α of falsely claiming its presence | VIM |
| error | (1) measured quantity value minus a reference quantity value<br>(2) difference of quantity value obtained by measurement and true value of the measurand<br>(3) difference of forecast value and a, estimate of the true value | VIM<br>CEOS |
| fiducial reference measurement | independent, fully characterised, and traceable (to a community agreed reference, ideally SI) measurement, tailored specifically to address the calibration/validation needs of satellite borne instruments making measurements of a particular measurand, that follow the guidelines outlined by the GEO/CEOS Quality Assurance framework for Earth Observation (QA4EO) | Goryl et al., (2023) |
| field-of-regard | an area of the object space scanned by the field-of-view of a scanning sensor | NIST |
| field-of-view | the solid angle from which the detector receives radiation | NIST |

| TERM | DEFINITION | SOURCE |
|---|---|---|
| footprint | the area of a target encircled by the field-of-view of a detector of radiation, or irradiated by an active system | NIST |
| influence quantity | quantity that, in a direct measurement, does not affect the quantity that is actually measured, but affects the relation between the indication and the measurement result | VIM |
| in situ measurement | (1) a direct measurement of the measurand in its original place<br>(2) any sub-orbital measurement of the measurand | GEOSS |
| Level-0 data | reconstructed, unprocessed instrument and payload data at full resolution (atmospheric and calibration modes, housekeeping data), with any and all measurement and communications artefacts | |
| Level-1a data | reconstructed, unprocessed data at full resolution, time referenced, and annotated with ancillary information, including radiometric and geometric calibration coefficients and geo-referencing parameters (e.g., ephemeris) computed and appended but not applied to the Level 0 data | |
| Level-1b data | calibrated, geo-located Earth reflectance and radiance spectra in all spectral bands; solar irradiance data, annotation data and references to used calibration data | |
| Level-2 data | geophysical measurand at the same resolution and geolocation as the Level 1 source data from which it is derived | |
| Level-3 data | data or retrieved geophysical parameters (i.e. derived from Level 1 or 2 data products) mapped on uniform space-time grid scales, usually with some completeness and consistency. Such re-sampling may include averaging, compositing, kriging, use of Kalman filters… | |
| Level-4 data | model output or results from analyses of lower level data, i.e., parameters that are not directly measured by the instruments, but are derived from these measurements | |
| measurand | quantity intended to be measured | VIM |
| metadata | data about the data; parameters that describe, characterise, and/or index the data | WMO |
| monitoring | (1) systematic evaluation over time of some quantity<br>(2) by extension, evaluation over time of the performance of a system, of the occurrence of an event etc. | NIST |
| point-to-area (point-to-volume) representativeness | the probability that a point measurement lies within a specific range of area-average (volume-average) concentration value | Nappo |
| precision | closeness of agreement between quantity values obtained by replicate measurements of a quantity on the same or similar object under specified conditions | VIM |
| process validation | establishing documented evidence of a high degree of assurance that a specific process will consistently produce a product meeting its pre-determined specifications and quality characteristics | CDRH |
| quality assessment (QA) | QA refers to the overall management of the processes involved in obtaining the data | CEOS |
| quality control (QC) | QC refers to the activities undertaken to check and optimise accuracy and precision of the data after its collection | CEOS |

| TERM | DEFINITION | SOURCE |
|---|---|---|
| quality indicator (QI) | a means of providing a user of data or derived product with sufficient information to assess its suitability for a particular application. This information should be based on a quantitative assessment of its traceability to an agreed reference or measurement standard (ideally SI), but can be presented as a numeric or a text descriptor, provided the quantitative linkage is defined. | QA4EO |
| radiometric calibration | a determination of radiometric instrument performance in the spatial, spectral, and temporal domains in a series of measurements, in which its output is related to the true value of the measured radiometric quantity | NIST |
| random error | component of measurement error that in replicate measurements varies in an unpredictable manner; note that random measurement error equals measurement error minus systematic measurement error | VIM |
| relative standard uncertainty | standard measurement uncertainty divided by the absolute value of the measured quantity value | VIM |
| repeatability | measurement precision under set of conditions including the same measurement procedure, same operator, same measuring system, same operating conditions and same location, and replicated measurements over a short period of time | VIM |
| representativeness | the extent to which a set of measurements taken in a given space-time domain reflect the actual conditions in the same or different space-time domain taken on a scale appropriate for a specific application | Nappo |
| reproducibility | measurement precision under a set of conditions including different locations, operators, and measuring systems | VIM |
| resolution | (1) the least angular/linear/temporal/spectral distance between two identical point sources of radiation that can be distinguished according to a given criterion<br>(2) the least vertical/geographical/temporal distance between two identical atmospheric features that can be distinguished in a gridded numerical product or in time series of measurements; resolution is equal to or coarser than vertical/geographical/temporal sampling of the grid or the measurement time series | NIST |
| stability | ability of a measuring system to maintain its metrological characteristics constant with time | VIM |
| systematic error | component of measurement error that in replicate measurements remains constant or varies in a predictable manner | VIM |
| traceability | property of a measurement result relating the result to a stated metrological reference (free definition and not necessarily SI) through an unbroken chain of calibrations of a measuring system or comparisons, each contributing to the stated measurement uncertainty | VIM |

| TERM | DEFINITION | SOURCE |
|---|---|---|
| tropopause | the region of the atmosphere where the environmental temperature lapse rate changes from positive (in the troposphere) to negative (in the stratosphere)<br>the lowest level at which the lapse rate decreases to 2 °C/km or less, provided that the average lapse rate between this level and all higher levels within 2 km does not exceed 2 °C/km<br>occasionally, a second tropopause may be found if the lapse rate above the first tropopause exceeds 3 °C/km | WMO |
| uncertainty | non-negative parameter that characterizes the dispersion of the quantity values that are being attributed to a measurand, based on the information used | VIM |
| validation | (1) the process of assessing, by independent means, the quality of the data products derived from the system outputs<br>(2) verification where the specified requirements are adequate for an intended use<br>(3) the process of assessing, by independent means, the degree of correspondence between the value of the radiometric quantity derived from the output signal of a calibrated radiometric device and the actual value of this quantity.<br>(4) confirmation by examination and provision of objective evidence that specifications conform to user needs and intended uses, and that the particular requirements implemented through software can be consistently fulfilled | CEOS<br>VIM<br>NIST<br>CDRH |
| verification | (1) the provision of objective evidence that a given data product fulfils specified requirements; note that, when applicable, measurement uncertainty should be taken into consideration.<br>(2) the provision of objective evidence that the design outputs of a particular phase of the software development life cycle meet all of the specified requirements for that phase | VIM<br>CDRH |

## 7.2. Abbreviations and acronyms

| | |
|---|---|
| AD | Applicable Document |
| AK | Averaging Kernel |
| AMF | Air Mass Factor, or optical enhancement factor |
| ATBD | Algorithm Theoretical Basis Document |
| BIPM | Bureau International des Poids et Mesures |
| BIRA-IASB | Belgian Institute for Space Aeronomy |
| CCI | ESA's Climate Change Initiative programme |
| CDRH | Center for Devices and Radiological Health |
| CEOS | Committee on Earth Observation Satellites |
| CMUG | Climate Modelling User Group |
| CRG | Climate Research Group |
| DARD | Data Access Requirement Document |
| DFS | Degree of Freedom of the System |

| | |
|---|---|
| DHF | Data Host Facility |
| DOAS | Differential Absorption Optical Spectroscopy |
| DU | Dobson Unit – unit of vertical column density (2.69 $10^{16}$ molec.$cm^{-2}$) |
| EC | European Commission |
| Envisat | ESA's Environmental Satellite, launched March 1, 2002 |
| EO | Earth Observation |
| EOST | Earth Observation Science Team |
| ERS-2 | ESA's Earth Remote Sensing satellite 2, launched April 21, 1995 |
| ESA | European Space Agency |
| ESRIN | European Space Research Institute |
| EUMETSAT | European Organisation for the Exploitation of Meteorological Satellites |
| FTIR | Fourier Transform Infra-Red |
| GAW | WMO's Global Atmosphere Watch |
| GCOS | Global Climate Observing System |
| GEOSS | Global Earth Observation System of Systems |
| GOME | Global Ozone Monitoring Experiment |
| GUM | Guide to the expression of uncertainty in a measurement |
| ISO | International Organization for Standardization |
| JCGM | Joint Committee for Guides in Metrology |
| KNMI | Royal Dutch Meteorological Institute |
| Lidar | Light detection and ranging |
| MAX-DOAS | Multi Axis Differential Optical Absorption Spectroscopy |
| MetOp | EUMETSAT's Meteorological Operational satellite |
| MPC | Mission Performance Centre |
| NDACC | Network for the Detection of Atmospheric Composition Change |
| OMI | Ozone Monitoring Instrument |
| Pandora | not an acronym; direct Sun UV-visible spectrometer |
| PVP | Product Validation Plan |
| QA4EO | Quality Assurance framework for Earth Observation |
| RD | Reference Document |
| S5P | Sentinel-5 Precursor |
| SCIAMACHY | SCanning Imaging Absorption spectroMeter for Atmospheric CHartographY |
| SZA | Solar Zenith Angle |
| TCCON | Total Carbon Column Observing Network |
| TROPOMI | TROPOspheric Monitoring Instrument |
| ULB | Université Libre de Bruxelles |
| URD | User Requirement Document |
| UT | Upper Troposphere |
| VALT | Validation team of the Ozone_cci project |
| VIM | International Vocabulary of Metrology |
| WGCV | CEOS Working Group on Calibration and Validation |
| WMO | World Meteorological Organization |
| ZSL-DOAS | Zenith-scattered-light Differential Optical Absorption Spectroscopy |

## 7.3. Validation metadata

To facilitate proper interpretation and consolidation of the validation results, documentation of the validation process is essential. Therefore, validation metadata, that is, brief but unambiguous documentation of the entire validation process leading to a validation graph or a comparison data file, should accompany any validation result reported in the PVIR and PVASR. Where validation results are provided in graphical format, validation metadata can be provided in a legend placed on the graph itself or below; they can also be attached to the graphical file as a *readme.file.text*. Where validation results are provided in numerical format (e.g., in an ASCII, HDF or NetCDF file), validation metadata can be included in this numerical data file as a header or simply attached externally to the file.

The metadata on the validation process must provide a short, unambiguous description of the comparison manipulations undertaken to obtain the validation results. From this information one should be able to check if the validation process complies with agreed standards and best practices. The step-by-step description of the data manipulations should also allow proper interpretation of the comparison results and further investigation of the data quality.

Table 21 describes the information that should be available in the validation metadata to ensure traceability of the validation process. Ideally it should not duplicate information that is already available, e.g., in the metadata accompanying the data under evaluation and the validation source.

**Table 21. Suggested validation metadata**

| VALIDATION STEP / ITEM | DETAILS |
|---|---|
| High-level description of the content of validation results (graphic file or numerical data file) | Identification of the data being validated and of the reference data used as a validation source, date, basic description of the results being reported |
| Metadata on data under evaluation | Data processing and archiving centre, model or data processor version, input and initialisation data, native data format (e.g., number density or volume mixing ratio, versus altitude or pressure…), data file name (at least file name convention) |
| Metadata on reference data used as a validation source | Data processing and archiving centre, instrument, responsible institute, model/data processor version, calibration version (input level-1 data), measured parameter, native data format… |
| Traceability of validation process | Step-by-step description of the data manipulations: data selection, conversion of units, filtering based, e.g., on flags or statistical tests, co-location criteria (vertical, horizontal and temporal), re-gridding and smoothing (vertical and horizontal, e.g. using a Gaussian, averaging kernels etc.), domain of the comparisons (geographical, vertical, temporal), reference to an agreed reference practice… |
| Format of validation results | Content of the numerical validation data file or description of the information displayed on the validation graph: units, relative or absolute difference, individual comparison pair or monthly mean, amount of comparison events, statistical estimators (mean/deviation or median/interpercentile) … |
| Credit and responsibilities | Analysis carried out at institute X by validation scientist Y supported by data processing scientist Z, contact (email)… |

END OF DOCUMENT