ECMWF COPERNICUS REPORT

Copernicus Climate Change Service

Product Quality Assessment Report (PQAR) – Main document for Greenhouse Gas (GHG: CO_2 & CH_4) data set CDR6 (01.2003-12.2021)

C3S2_312a_Lot2_DLR – Atmosphere

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History of modifications

Version	Date	Description of modification	Chapters / Sections
1.3	20-October-2017	New document for data set CDR1 (temporal coverage: 2003-2016)	All
2.0	16-October-2018	Update for data set CDR2 (temporal coverage: 2003-2017)	All
3.0	12-August-2019	Update for data set CDR3 (temporal coverage: 2003-2018)	All
4.0	17-September-2020	Update for data set CDR4 (temporal coverage: 2003-2019)	All
5.0	23-April-2021	Update for data set CDR5 (temporal coverage: 2003-mid2020)	All
6.0	04-August-2022	Update for data set CDR6 (temporal coverage: 2003-2021)	All
6.1	14-December-2022	Update after review (use of new template, several improvements at various places)	All
6.2	30-January-2023	Update after 2nd review. Several improvements at various places.	All
6.3	02-March-2023	Clean version after 2nd review. Minor improvements at various places.	All

List of datasets covered by this document

Deliverable ID	Product title (*)	Product type (CDR, ICDR)	Version number	Delivery date
WP2-FDDP-GHG-v1	CO2_GOS_OCFP (ANNEX A)	CDR 6	7.3	31-Aug-2022
WP2-FDDP-GHG-v1	CH4_GOS_OCFP (ANNEX A)	CDR 6	7.3	31-Aug-2022
WP2-FDDP-GHG-v1	CH4_GOS_OCPR (ANNEX A)	CDR 6	9.0	31-Aug-2022
WP2-FDDP-GHG-v1	CO2_GO2_SRFP (ANNEX B)	CDR 6	2.0.0	31-Aug-2022
WP2-FDDP-GHG-v1	CH4_GO2_SRFP (ANNEX B)	CDR 6	2.0.0	31-Aug-2022
WP2-FDDP-GHG-v1	CH4_GO2_SRPR (ANNEX C)	CDR 6	2.0.0	31-Aug-2022
WP2-FDDP-GHG-v1	XCO2_EMMA, XCH4_EMMA, XCO2_OBS4MIPS, XCH4_OBS4MIPS (ANNEX D)	CDR 6	4.4	31-Aug-2022
WP2-FDDP-GHG-v1	CO2_IASA_NLIS, CH4_IASA_NLIS, CO2_IASB_NLIS, CH4_IASB_NLIS (ANNEX E) (#)	CDR 6	9.1	31-Aug-2022

(*) In brackets: see listed ANNEX to this MAIN document for details on listed product(s).
(#) ANNEX E also includes some information on product CO2_AIRS_NLIS (v3.0) but that product has been generated in a pre-cursor project and no assessments have been carried out in this project. Therefore, this product is not listed here.

Related documents

Reference ID	Document
D1	**GCOS-154:** Global Climate Observing System (GCOS): SYSTEMATIC OBSERVATION REQUIREMENTS FOR SATELLITE-BASED DATA PRODUCTS FOR CLIMATE - 2011 Update - Supplemental details to the satellite-based component of the "Implementation Plan for the Global Observing System for Climate in Support of the UNFCCC (2010 Update)", December 2011, prepared by World Meteorological Organization (WMO), Intergovernmental Oceanographic Commission, United Nations Environment Programme (UNEP), International Council for Science, Doc.: GCOS 154, link: http://cci.esa.int/sites/default/files/gcos-154.pdf, 2011.
D2	**GCOS-200:** The Global Observing System for Climate: Implementation Needs, World Meteorological Organization (WMO), GCOS-200 (GOOS-214), pp. 325, link: http://unfccc.int/files/science/workstreams/systematic_observation/application/pdf/gcos_ip_10oct2016.pdf, 2016.
D3	**ESA-CCI-GHG-URDv2.1:** Chevallier, F., et al., User Requirements Document (URD), ESA Climate Change Initiative (CCI) GHG-CCI project, Version 2.1, 19 Oct 2016, https://www.iup.uni-bremen.de/carbon_ghg/docs/GHG-CCIplus/URD/URDv2.1_GHG-CCI_Final.pdf, 2016.
D4	**TRD GAD GHG, 2021:** Buchwitz, M., Reuter, M., Schneising-Weigel, O., Aben, I., Wu, L., Hasekamp, O. P., Boesch, H., Di Noia, A., Crevoisier, C., Armante, R.: Target Requirement and Gap Analysis Document, Copernicus Climate Change Service (C3S) project on satellite-derived Essential Climate Variable (ECV) Greenhouse Gases (CO_2 and CH_4) data products, Version 3.1, 19-February-2021, pp. 81, 2021. Latest version: http://wdc.dlr.de/C3S_312b_Lot2/Documentation/GHG/C3S2_312a_Lot2_TRD-GAD_GHG_latest.pdf
D5	**ATBD GHG, 2023:** Buchwitz, M., Barr, A., Boesch, H., Borsdorff, T., Crevoisier, C., Di Noia, A., Hasekamp, O. P., Landgraf, J., Meilhac, N., Parker, R., Reuter, M., Schneising-Weigel, O.: Algorithm Theoretical Basis Document (ATBD) – Main document for Greenhouse Gas (GHG: CO_2 & CH_4) data set CDR6 (01.2003-12.2021), C3S project C3S2_312a_Lot2_DLR, v6.3, 2023.
D6	**PUGS GHG, 2023:** Buchwitz, M., Barr, A., Boesch, H., Borsdorff, T., Crevoisier, C., Di Noia, A., Hasekamp, O. P., Landgraf, J., Meilhac, N., Parker, R., Reuter, M., Schneising-Weigel, O.: Product User Guide and Specification (PUGS) – Main document for Greenhouse Gas (GHG: CO_2 & CH_4) data set CDR6 (01.2003-12.2021), C3S project C3S2_312a_Lot2_DLR, v6.3, 2023.
D7	**PQAD GHG, 2023:** Buchwitz, M., Boesch, H., Borsdorff, T., Crevoisier, C., Di Noia, A., Hasekamp, O. P., Landgraf, J., Meilhac, N., Parker, R., Reuter, M., Schneising-Weigel, O.: Product Quality Assurance Document (PQAD) for Greenhouse Gas (GHG) CO_2 & CH_4) data set Climate Data Record No. 6 (CDR6, 01.2003-12.2021), C3S project C3S2_312a_Lot2_DLR, v6.3, 2023.

Acronyms

Acronym	Definition
AIRS	Atmospheric Infrared Sounder
AMSU	Advanced Microwave Sounding Unit
ATBD	Algorithm Theoretical Basis Document
BESD	Bremen optimal EStimation DOAS
CAR	Climate Assessment Report
C3S	Copernicus Climate Change Service
CCDAS	Carbon Cycle Data Assimilation System
CCI	Climate Change Initiative
CDR	Climate Data Record
CDS	(Copernicus) Climate Data Store
CMUG	Climate Modelling User Group (of ESA's CCI)
CRG	Climate Research Group
D/B	Data base
DOAS	Differential Optical Absorption Spectroscopy
EC	European Commission
ECMWF	European Centre for Medium Range Weather Forecasting
ECV	Essential Climate Variable
EMMA	Ensemble Median Algorithm
ENVISAT	Environmental Satellite (of ESA)
EO	Earth Observation
ESA	European Space Agency
EU	European Union
EUMETSAT	European Organisation for the Exploitation of Meteorological Satellites
FCDR	Fundamental Climate Data Record
FoM	Figure of Merit
FP	Full Physics retrieval method
FTIR	Fourier Transform InfraRed
FTS	Fourier Transform Spectrometer
GCOS	Global Climate Observing System
GEO	Group on Earth Observation
GEOSS	Global Earth Observation System of Systems
GHG	GreenHouse Gas
GHG-CCI	GHG project of ESA's CCI
GOME	Global Ozone Monitoring Experiment
GMES	Global Monitoring for Environment and Security
GOSAT	Greenhouse Gases Observing Satellite
GOSAT-2	Second GOSAT satellite

IASI	Infrared Atmospheric Sounding Interferometer
IMAP-DOAS (or IMAP)	Iterative Maximum A posteriori DOAS
IPCC	International Panel in Climate Change
IUP	Institute of Environmental Physics (IUP) of the University of Bremen, Germany
JAXA	Japan Aerospace Exploration Agency
JCGM	Joint Committee for Guides in Metrology
L1	Level 1
L2	Level 2
L3	Level 3
L4	Level 4
LMD	Laboratoire de Météorologie Dynamique
MACC	Monitoring Atmospheric Composition and Climate, EU GMES project
NA	Not applicable
NASA	National Aeronautics and Space Administration
NetCDF	Network Common Data Format
NDACC	Network for the Detection of Atmospheric Composition Change
NIES	National Institute for Environmental Studies
NIR	Near Infra Red
NLIS	LMD/CNRS *neuronal* network mid/upper tropospheric CO2 and CH4 retrieval algorithm
NOAA	National Oceanic and Atmospheric Administration
Obs4MIPs	Observations for Climate Model Intercomparisons
OCO	Orbiting Carbon Observatory
OE	Optimal Estimation
PBL	Planetary Boundary Layer
ppb	Parts per billion
ppm	Parts per million
PR	(light path) PRoxy retrieval method
PUGS	Product User Guide and Specification
PVIR	Product Validation and Intercomparison Report
QA	Quality Assurance
QC	Quality Control
REQ	Requirement
RMS	Root-Mean-Square
RTM	Radiative transfer model
SCIAMACHY	SCanning Imaging Absorption spectroMeter for Atmospheric ChartographY
SCIATRAN	SCIAMACHY radiative transfer model
SRON	SRON Netherlands Institute for Space Research
SWIR	Short Wava Infra Red
TANSO	Thermal And Near infrared Sensor for carbon Observation

TANSO-FTS	Fourier Transform Spectrometer on GOSAT
TANSO-FTS-2	Fourier Transform Spectrometer on GOSAT-2
TBC	To be confirmed
TBD	To be defined / to be determined
TCCON	Total Carbon Column Observing Network
TIR	Thermal Infra Red
TR	Target Requirements
TRD	Target Requirements Document
WFM-DOAS (or WFMD)	Weighting Function Modified DOAS
UoL	University of Leicester, United Kingdom
URD	User Requirements Document
WMO	World Meteorological Organization
Y2Y	Year-to-year (bias variability)

General definitions

Essential climate variable (ECV)

An ECV is a physical, chemical, or biological variable or a group of linked variables that critically contributes to the characterization of Earth's climate.

Climate data record (CDR)

The US National Research Council (NRC) defines a CDR as a time series of measurements of sufficient length, consistency, and continuity to determine climate variability and change.

Fundamental climate data record (FCDR)

A fundamental climate data record (FCDR) is a CDR of calibrated and quality-controlled data designed to allow the generation of homogeneous products that are accurate and stable enough for climate monitoring.

Thematic climate data record (TCDR)

A thematic climate data record (TCDR) is a long time series of an essential climate variable (ECV).

Intermediate climate data record (ICDR)

An intermediate climate data record (ICDR) is a TCDR which undergoes regular and consistent updates, for example because it is being generated by a satellite sensor in operation.

Satellite data processing levels

The NASA Earth Observing System (EOS) distinguishes six processing levels of satellite data, ranging from Level 0 (L0) to Level 4 (L4) as follows.

L0	Unprocessed instrument data
L1A	Unprocessed instrument data alongside ancillary information
L1B	Data processed to sensor units (geo-located calibrated spectral radiance and solar irradiance)
L2	Derived geophysical variables (e.g., XCO_2) over one orbit
L3	Geophysical variables averaged in time and mapped on a global longitude/latitude horizontal grid
L4	Model output derived by assimilation of observations, or variables derived from multiple measurements (or both)

Additional definitions as relevant for this document:

In the following some relevant Target Requirement (TR) related definitions are given. For details please see *TRD (D4), 2017*, *ESA-CCI-GHG-URDv2.1* and *CMUG-RBD, 2010*:

Systematic error: component of measurement error that in replicate measurements remains constant or varies in a predictable manner

Note: "Systematic error" = "Absolute systematic error" (in contrast to "Relative systematic error" defined below).

For satellite GHG ECV products especially the "Relative systematic error" is important. The definition as used here is as follows:

Relative systematic error: Identical with "Systematic error" but after bias correction and without considering a possible "global offset" (overall mean bias). Reflects the importance of spatially and temporally correlated errors ("spatio-temporal biases"). Computed from standard deviations of spatial and temporal biases.

Bias: estimate of a systematic measurement error (*JCGM, 2008*).

Precision is the measure of reproducibility or repeatability of the measurement without reference to an international standard so that precision is a measure of the random and not the systematic error. Suitable averaging of the random error can improve the precision of the measurement but does not establish the systematic error of the observation (*CMUG-RBD, 2010*).

Note: Precision (as explained in *TRD (D4)*) is quantified with the standard deviation (1-sigma) of the error distribution.

Stability is a term often invoked with respect to long-term records when no absolute standard is available to quantitatively establish the systematic error - the bias defining the time-dependent (or instrument-dependent) difference between the observed quantity and the true value (*CMUG-RBD, 2010*).

Note: Stability requirements cover inter-annual error changes. If the change in the average bias from one year to another is larger than the defined values, the corresponding product does not meet the stability requirement.

Representativity is important when comparing with or assimilating in models. Measurements are typically averaged over different horizontal and vertical scales compared to model fields. If the measurements are smaller scale than the model it is important. The sampling strategy can also affect this term (*CMUG-RBD, 2010*).

Threshold requirement: The threshold is the limit at which the observation becomes ineffectual and is not of use for climate-related applications (*CMUG-RBD, 2010*).

Goal requirement: The goal is an ideal requirement above which further improvements are not necessary (*CMUG-RBD, 2010*).

Breakthrough requirement: The breakthrough is an intermediate level between the "threshold" and "goal"requirements, which - if achieved - would result in a significant improvement for the targeted application. The breakthrough level may be considered as an optimum, from a cost-benefit point of view when planning or designing observing systems (*CMUG-RBD, 2010*).

Horizontal resolution is the area over which one value of the variable is representative of (*CMUG-RBD, 2010*).

Vertical resolution is the height over which one value of the variable is representative of. Only used for profile data (*CMUG-RBD, 2010*).

Observing Cycle (or **Revisit Time**) is the temporal frequency at which the measurements are required (*CMUG-RBD, 2010*).

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Scope of document

This document is the Product Quality Assessment Report (PQAR) for the Copernicus Climate Change Service (C3S, https://climate.copernicus.eu/) component as covered by the greenhouse gas (GHG) sub-project of project C3S2_312a_Lot2 led by DLR, Germany (a follow-on activity of project C3S_312b_Lot2 led by DLR and project C3S_312a_Lot6 led by University of Bremen, Germany), in the following referred to as C3S/GHG project or simply as project.

Within this project satellite-derived atmospheric carbon dioxide (CO_2) and methane (CH_4) Essential Climate Variable (ECV) data products have been generated and provided to ECMWF for inclusion into the Copernicus Climate Data Store (CDS) from which users can access these data products and the corresponding documentation.

The satellite-derived data products described and quality assessed in this document are:

- Column-averaged dry-air mixing ratios (mole fractions) of CO_2 and CH_4, denoted XCO_2 (in parts per million, ppm) and XCH_4 (in parts per billion, ppb), respectively.
- Mid/upper tropospheric mixing ratios of CO_2 (in ppm) and CH_4 (in ppb).

An overview about the products is given in Table 1 for the CO_2 products and in Table 2 for the CH_4 products.

Requirements on data quality are formulated in the corresponding Target Requirement and Gap Analysis Document (TRGAD) (*D4*).

The main purpose of this document is to describe the validation / quality assessment of the satellite-derived CO_2 and CH_4 greenhouse gas (GHG) ECV data products.

The product validation methodology is identical with the methodology as described in the Product Quality Assurance Document (PQAD) (*D7*). This methodology is also described in this PQAR document so that this document contains all relevant information and users do not have to read document PQAD in addition to this PQAR document.

Note that the product validation methodology only describes the high-level validation procedure and main quantities to be computed (e.g., random and systematic errors, etc.) but that validation protocol does not define all details (such as which spatial and temporal colocation criteria to use) to avoid overspecification. Note that more than one validation approach has been used for most products to obtain robust validation results. These different approaches all follow the general validation methodology but differ in several aspects, which are (on purpose) not prescribed by the validation methodology in order to obtain a small ensemble of validation approaches and corresponding validation results.

For all XCO_2 and XCH_4 products three validation approaches are used. One of these methods is called “QA/QC approach” (see Reuter et al., 2020) and this approach has been applied to all XCO_2

and XCH_4 products and detailed results are reported in this Main PQAR document. The second approach is called "EMMA approach" (see also Reuter et al., 2020) and has also been applied to all XCO_2 and XCH_4 products. In addition, each data provider has also carried out a validation using his/her "data provider approach" as applied to their product or groups of products. These data provider validation results and the EMMA validation results are described in 5 ANNEXes to this MAIN PQAR document:

- ANNEX A: PQAR for products CO2_GOS_OCFP, CH4_GOS_OCFP, CH4_OCPR (University of Leicester's GOSAT products)
- ANNEX B: PQAR for products CO2_GO2_SRFP, CH4_GO2_SRFP (SRON's "full physics" GOSAT-2 products)
- ANNEX C: PQAR for product CH4_GO2_SRPR (SRON's "proxy" GOSAT-2 XCH_4 product)
- ANNEX D: PQAR for products XCO2_EMMA, XCH4_EMMA, XCO2_OBS4MIPS, XCH4_OBS4MIPS (University of Bremen's merged Level 2 and Level 3 products)
- ANNEX E: PQAR for IASI CO_2 and CH_4 products and AIRS CO_2 product (LMD/CNRS's IASI and AIRS products)

This MAIN PQAR document describes in detail the validation results as obtained using the QA/QC approach and summarizes the results from other validation approaches. All validation results are combined to obtain the overall validation summary results. This ensemble validation approach has been used in order to obtain robust validation results.

Table 1: Overview CO_2 products. "CRD#" indicates the Climate Data Record Number. Level 2 (L2) products contains information for each individual satellite footprint (ground pixel) whereas Level 3 (L3) products are gridded /averaged spatially and temporally.

Product ID (Level)	Version	CDR#	Temporal coverage	Comments
CO2_GOS_OCFP (L2)	7.3	4-6	04.2009 – 12.2021	XCO_2 from GOSAT as retrieved with Univ. Leicester's OCFP algorithm.
CO2_GO2_SRFP (L2)	2.0.0	6	02.2019 – 12.2021	XCO_2 from GOSAT-2 as retrieved with SRON's SRFP (RemoTeC) algorithm.
XCO2_EMMA (L2)	4.4	6	01.2003 – 12.2021	Merged L2 XCO_2 product using Univ. Bremen's EMMA algorithm.
XCO2_OBS4MIPS (L3)	4.4	6	01.2003 – 12.2021	Merged L3 XCO_2 product in OBS4MIPS format.
CO2_IASA_NLIS (L2)	9.1	4-6	07.2007 – 08.2021	Mid-tropospheric CO_2 mixing ratios as retrieved from IASI/Metop-A using LMD's NLIS algorithm.
CO2_IASB_NLIS (L2)	9.1	4-6	02.2013 – 12.2021	Mid-tropospheric CO_2 mixing ratios as retrieved from IASI/Metop-B using LMD's NLIS algorithm.

Table 2: Overview CH_4 products. "CRD#" indicates the Climate Data Record Number. Level 2 (L2) products contains information for each individual satellite footprint (ground pixel) whereas Level 3 (L3) products are gridded /averaged spatially and temporally.

Product ID (Level)	Version	CDR#	Temporal coverage	Comments
CH4_GOS_OCFP (L2)	7.3	4-6	04.2009 – 12.2021	XCH_4 from GOSAT as retrieved with Univ. Leicester's OCFP algorithm.
CH4_GOS_OCPR (L2)	9.0	4-6	04.2009 – 12.2021	XCH_4 from GOSAT as retrieved with Univ. Leicester's OCPR algorithm.
CH4_GO2_SRFP (L2)	2.0.0	6	02.2019 – 12.2021	XCH_4 from GOSAT-2 as retrieved with SRON's SRFP (RemoTeC) algorithm.
CH4_GO2_SRPR (L2)	2.0.0	6	02.2019 – 12.2021	XCH_4 from GOSAT-2 as retrieved with SRON's SRPR (RemoTeC) algorithm.
XCH4_EMMA (L2)	4.4	6	01.2003 – 12.2021	Merged L2 XCH_4 product using Univ. Bremen's EMMA algorithm.
XCH4_OBS4MIPS (L3)	4.4	6	01.2003 – 12.2021	Merged L3 XCH_4 product in OBS4MIPS format.
CH4_IASA_NLIS (L2)	9.1	4-6	07.2007 – 08.2021	Mid-tropospheric CH_4 mixing ratios as retrieved from IASI/Metop-A using LMD's NLIS algorithm.
CH4_IASB_NLIS (L2)	9.1	4-6	02.2013 – 12.2021	Mid-tropospheric CH_4 mixing ratios as retrieved from IASI/Metop-B using LMD's NLIS algorithm.

Executive summary

In this document the validation / quality assessment of satellite-derived atmospheric carbon dioxide (CO_2) and methane (CH_4) Climate Data Record (CDR) data products as generated via the C3S2_312a_Lot2 project of the Copernicus Climate Change Service (C3S, https://climate.copernicus.eu/) is described.

These satellite-derived greenhouse gas (GHG) data products are:

- Column-averaged dry-air mixing ratios (mole fractions) of CO_2 and CH_4, denoted XCO_2 (in parts per million, ppm) and XCH_4 (in parts per billion, ppb), respectively.
- Mid/upper tropospheric mixing ratios of CO_2 (in ppm) and CH_4 (in ppb).

The C3S GHG data products are generated from the satellite instruments SCIAMACHY/ENVISAT, TANSO-FTS/GOSAT, TANSO-FTS-2/GOSAT-2 (XCO_2 and XCH_4 products) and AIRS and IASI (mid/upper troposphere products). All data products are available as Level 2 (individual ground pixels) products. The XCO_2 and XCH_4 Level 2 products correspond to individual satellite sensors but are also available as merged multi-sensor products. In addition, also merged Level 3 (i.e., gridded) products in Obs4MIPs format are available for the XCO_2 and XCH_4 products. For details on data format etc. please see the Product User Guide and Specification (PUGS) document (PUGS, D6).

CO_2 and CH_4 are important climate-relevant atmospheric gases, so-called greenhouse gases (GHG). Because of their important role for climate, they are classified as Essential Climate Variables (ECVs). The ECV GHG as formulated by GCOS (Global Climate Observing System) is defined as: “Retrievals of greenhouse gases, such as CO_2 and CH_4, of sufficient quality to estimate regional sources and sinks” (GCOS-154). This definition contains already the main application of these atmospheric data products, namely to use them (in combination with appropriate (inverse) modelling) to obtain (improved) information on their (primarily surface) sources and sinks.

Both gases, CO_2 and CH_4, have a long lifetime in the atmosphere. As a consequence of this fact and related human emissions the atmospheric concentrations of these gases are relatively high compared to other atmospheric trace gases. As a result of this, even a moderate to strong (surface) source or sink typically only results in a relatively small local or regional change (enhancement or depletion relative to the surrounding region) in their vertical columns or their mid/upper tropospheric concentration. The observational requirements are therefore very demanding in particular with respect to random and systematic errors and stability.

Because of their long lifetime and atmospheric transport, elevated (or depleted) atmospheric CO_2 and CH_4 concentrations can be higher (or lower) relative to the background far away from the surface source (or sink), which has emitted (or taken up) these atmospheric gases. In order to obtain source/sink information from the atmospheric observations it is therefore required to take atmospheric transport (and in particular for methane also atmospheric chemistry) into account and to consider the exact time and location of the atmospheric observations. As a consequence, the most relevant data products are the Level 2 (L2) products, which contain detailed information (time, location, etc.) for each individual satellite ground pixel. The requirements as formulated in the

Target Requirement and Gap Analysis Document (TRGAD, D4) are, therefore, mostly L2 requirements. However, for XCO_2 and XCH_4 also (gridded) Level 3 (L3) products have been generated (in Obs4MIPs format) and also their validation is described in this document.

The product validation methodology is identical with the methodology as described in the Product Quality Assurance Document (PQAD) (D7). This methodology is also described in this PQAR document so that this document contains all relevant information and users do not have to read document PQAD in addition to this PQAR document.

The product validation results can be summarized as follows:

Summary quality Level 2 XCO_2 products:

The achieved single observation random error (or precision) is typically close to 2 ppm and better than 3 ppm for all products. This is better than the required breakthrough requirement (B) of better than 3 ppm but somewhat worse than the goal (G) requirement of better than 1 ppm.

The systematic error (relative accuracy) threshold (T) requirement is “better than 0.5 ppm”. The achieved performance is around 0.7 ppm +/- a few 0.1 ppm, depending on product and assessment method. The probability that the threshold requirement is met is 44% for product CO2_GOS_OCFP, 21% for CO2_GO2_SRFP and 77% for XCO2_EMMA.

Stability is very good. No significant linear bias drift has been detected. The probability that the threshold (T) stability requirement of 0.5 ppm/year is met is close to 100% percent for all product except for product CO2_GO2_SRFP (61%).

Summary quality Level 2 XCH_4 products:

The achieved single observation random error (or precision) is close to 17 ppb, which is the breakthrough (B) requirement, for the GOSAT and the EMMA products. For product CH4_GO2_SRFP the precision is near 20 ppb and for product CH4_GO2_SRPR the precision is slightly larger than 20 ppb.

The systematic error (relative accuracy) threshold (T) requirement is “better than 10 ppb”. The achieved performance is around 5 ppb for the GOSAT and the EMMA products and product CH4_GO2_SRFP. For product CH4_GO2_SRPR the estimated accuracy depends on assessment method and is in the range 5 – 10 ppb.

Stability is very good for all GOSAT products and the EMMA product. For these products no significant linear bias drift has been detected. The probability that the threshold (T) stability requirement of 3 ppb/year is met is close to 100% for these products. The probability is much less for the two GOSAT-2 products (58% for the FP product and 50% for the PR product, but note that these products only cover relatively short time periods).

Summary quality Level 3 XCO_2 product:

The validation of Level 3 product XCO2_OBS4MIPS can be summarized as follows: The overall monthly mean uncertainty is 1.1 ppm and the mean bias is 0.28 ppm. Relative systematic errors, i.e., spatial and temporal biases amount to 0.5±0.6 ppm. The computed linear drift of 0.09±0.23 ppm is small and not significant. The probability that the 0.5 ppm accuracy requirement is met is 68%. The probability that the 0.5 ppm/year stability requirement is met is 95%.
Overall, this product has therefore reasonable accuracy and high stability.

Summary quality Level 3 XCH_4 product:

The validation of product XCH4_OBS4MIPS can be summarized as follows: The overall monthly mean uncertainty is 7.9 ppb and the mean bias is 4.4 ppb. Relative systematic errors, i.e., spatial and temporal biases amount to 4.7±6 ppb. The computed linear drift of 0.45±1.2 ppb is small and not significant. The probability that the 10 ppb accuracy requirement is met is 89%. The probability that the 3 ppb/year stability requirement is met is 98%. Overall, this product has therefore very good accuracy and high stability.

Summary quality IASI mid-tropospheric Level 2 CO_2 products:

The single measurement precision of product CO2_IASA_NLIS (from IASI on Metop-A) is 1 ppm. The mean bias (global offset) is 0.96 ppm. The estimated relative accuracy is around 1 ppm. The probability that the < 0.5 ppm user requirement is met has been estimated to 50% taking into account the uncertainty of the reference data and assessment method. The product is also very stable (0.06 +/- 0.10 ppm/year (1-sigma)) meeting the requirement for long-term drift stability. The performance of product CO2_IASB_NLIS (from IASI on Metop-B) is similar.

Summary quality IASI mid-tropospheric Level 2 CH_4 products:

The single measurement precision of product CH4_IASA_NLIS (from IASI on Metop-A) is 12 ppb. The mean bias (global offset) is -3.4 ppb. The product appears to meet the “relative systematic error” requirement of better than 10 ppb: the estimated relative accuracy is 3.4 ppb. The product appears to be very stable but a quantitative analysis could not be carried out due to lack of reference data. The performance of product CH4_IASB_NLIS (from IASI on Metop-B) is similar.

1. Product validation methodology

The product validation methodology is identical with the methodology as described in the Product Quality Assurance Document (PQAD) (D7). This methodology is also described in this PQAR document so that this document contains all relevant information and users do not have to read document PQAD in addition to this PQAR document.

1.1 Description of reference data used for validation

1.1.1 Reference data for validation of the XCO_2 and XCH_4 Level 2 products

1.1.1.1 TCCON network

For validation of satellite XCO_2 and XCH_4 retrievals the Total Carbon Column Observing Network (TCCON, http://www.tccon.caltech.edu/) has been established (e.g., Wunch et al., 2010, 2011, 2015).

This network is the core network used for validation of the satellite XCO_2 and XCH_4 retrievals. Nevertheless, there are also some limitations as explained in Sect. 1.2.1.4.1.

TCCON provides XCO_2 and XCH_4 data products as retrieved from ground-based Fourier Transform Infrared (FTIR) observations based on direct sun observations. Currently, there are about 25 TCCON sites (see Sect. 1.2.1.4.1).

The TCCON data products can essentially be directly compared with the satellite-derived XCO_2 and XCH_4 data products and TCCON data products have been used for this purpose extensively in the past as shown in many studies and publications. A short overview about these activities is given in Sect. 1.2.1.1.

All previous validation results as documented in previous versions of this document were based on using TCCON version GGG2014 (e.g., Wunch et al., 2015). On 2022-04-27 an initial version of GGG2020 data was released (https://tccon-wiki.caltech.edu/Main/GGG2020DataChanges) (with some sites still missing). The QA/QC validation results shown in this document are based on GGG2020 (Laughner et al., 2021). Other validation results (e.g., those based on the EMMA method) are still based on GGG2014 (as data from more validation sites are available compared to GGG2020). As in previous assessments we assume that the uncertainty of the TCCON XCO_2 data product is 0.4 ppm (1-sigma) and that the XCH_4 uncertainty is 4 ppb (1-sigma).

1.1.1.2 Traceability to standard

As explained in this document, the satellite-derived XCO_2 and XCH_4 data products will be validated by comparison with TCCON XCO_2 and XCH_4 data products, which in turn have been calibrated

against the World Meteorological Organization (WMO) in situ trace gas measurement scales (see Wunch et al., 2010). This approach ensures that the satellite XCO_2 and XCH_4 retrievals are linked to the WMO standards for atmospheric CO_2 and CH_4 measurements.

1.1.2 Reference data for validation of the mid/upper tropospheric CO_2 and CH_4 products

1.1.2.1 Reference data overview

For validation of mid/upper tropospheric CO_2 and CH_4, no remote sensing ground-based measurements (such as TCCON) is available. Use is thus made of sparse airborne (aircrafts and balloons) measurements: averaging kernels associated to the retrieved columns are applied to vertical profiles measured by in-situ instruments and the resulting column is compared to columns measured from space.

Validation thus relies on:

- aircraft data acquired either during regular measurements on-board commercial airliners: CONTRAIL (https://www.cger.nies.go.jp/contrail/contrail.html), IAGOS (https://www.iagos.org/) in the future.
- aircraft regular measurements made by research groups: NOAA (https://www.noaa.gov/) aircraft network in the US and Canada.
- aircraft research campaigns: HIPPO (https://www.eol.ucar.edu/content/about-hippo), CoMet (https://www.halo.dlr.de/science/missions/comet/comet.html) in the future.
- Balloon measurements: AirCores (https://aircore.aeris-data.fr/) at various locations (Timmins, Kiruna, Sodankulä, Trainou-Orléans).

1.1.2.2 Traceability to standard

As explained in the following sections, the satellite mid/upper tropospheric CO_2 and CH_4 will be validated by comparison with aircraft and balloon measurements, which are calibrated against the World Meteorological Organization (WMO) scales. This ensures that the satellite retrievals are linked to WMO standards for atmospheric CO_2 and CH_4.

1.2 Description of product validation methodology

1.2.1 Methods for validation of XCO_2 and XCH_4 Level 2 products

In this section, the validation methodology is described. In the following sections the described methods are applied to the newly generated data sets.

1.2.1.1 Overview validation of GHG-CCI pre-cursor / pre-operational products

Past versions of satellite XCO_2 and XCH_4 retrievals as obtained from SCIAMACHY/ENVISAT and TANSO-FTS/GOSAT have been extensively validated using TCCON as described in various peer-reviewed scientific publications (e.g., Buchwitz et al., 2013a, 2016; Butz et al., 2010; Cogan et al., 2011; Dils et al., 2004; Parker et al., 2011; Reuter et al., 2011; Schneising et al., 2011; Yoshida et al., 2013), project related reports (e.g., Buchwitz et al., 2017) and other documents (e.g., Buchwitz et al., 2016a, 2017a; Reuter et al., 2016, 2017a).

The latest version of the satellite XCO_2 and XCH_4 retrievals as generated within the GHG-CCI project of ESA's Climate Change Initiative is called "Climate Research Data Package No. 4" (CRDP4). The quality assessment of that data set is described in the Product Validation and Intercomparison Report, version 5, PVIRv5 (Buchwitz et al., 2017). That GHG-CCI CRDP4 data set is the pre-cursor data set, which has been extended for C3S in the context of the C3S_312a_Lot6 project, a pre-cursor project of the current C3S project. As shown in document PVIRv5 (Buchwitz et al., 2017) the validation of the GHG-CCI CRDP4 pre-cursor XCO_2 and XCH_4 data products has been carried out by comparison with TCCON ground-based XCO_2 and XCH_4 retrievals. The assessments have been carried out quasi independently by different individuals / teams using (somewhat) different methods (using all or only a sub-set of the TCCON sites, using different criteria for spatio-temporal co-location, using different methods to compute "relative systematic error" and "year-to-year bias variability, using "direct comparison" or the Ensemble Median Algorithm (EMMA, Reuter et al., 2013) to check and ensure robustness of the findings. It had been found that quite similar overall quality assessment results have been obtained using the different methods (see PVIRv5 for details), i.e., robust conclusions have been obtained.

The quality assessment was based on the computation of several quantities (metrics). The most important ones are:

- Single ground pixel random error (or "single measurement precision", 1-sigma): Computed as the standard deviation of the difference of the single satellite measurement with TCCON.
- Mean bias (per site and globally): Computed as the mean difference of the satellite measurements with TCCON (satellite minus TCCON).
- "Relative systematic error" (or "relative accuracy" or "relative bias"): To estimate this quantity the "spatial bias" had been computed as standard deviation of the biases as obtained at the various individual TCCON sites. This value is reported in several peer-reviewed publications (e.g., Dils et al., 2014) but does not consider temporal biases. To

also address temporal biases Dils et al., 2014, also computed the quantities “seasonal mean bias”, “seasonality” and “seasonal relative accuracy” (SRA).
- Stability: Linear bias trend (drift): Computed from the slope (and the error of the slope) as obtained by fitting a straight line to satellite minus TCCON differences.
- Stability: Year-to-year bias variability: Computed as maximum minus minimum bias difference of smoothed (using a one year running average) satellite minus TCCON differences.

1.2.1.2 Data quality assessment methods

The quality assessments, which have been carried out for the newly generated C3S products, are similar as past assessments, which have been carried out for the pre-cursor products (see previous sub-section). However, there are some important differences, in particular those related to Target Requirements (TR) assessments, which have not been carried out for the pre-cursor products. The C3S assessment method is described in the following sub-sections.

1.2.1.2.1 Quantitative assessment methods

For each data product the following quantities have been determined:

Single ground pixel random error (or “single measurement precision”, 1-sigma):
Computed as the standard deviation of the difference of the single satellite retrievals (i.e., for individual ground pixels) with the co-located TCCON reference value. See also document PVIRv5 (Buchwitz et al., 2017) for an assessment of this quantity using the pre-cursor products.

Reported uncertainties (“Uncertainty ratio”):
The satellite-derived Level 2 XCO_2 and XCH_4 data products contain an uncertainty estimate for each single observation. This uncertainty is meant to be the statistical uncertainty (1-sigma, dominated by the random error component of the uncertainty due to instrument noise) associated with that single observation. To assess the quality of these uncertainty estimates they are compared with the standard deviation of satellite minus TCCON retrievals at the various TCCON sites. It is expected that the mean value of the reported uncertainty is similar in magnitude (agreement within a few 10%) as the standard deviation of the difference to TCCON (this should be the case if the reported uncertainty is correct and if the comparison method does not introduce additional errors). Therefore, one expects that the “Uncertainty ratio”, i.e., the ratio of the mean value of the reported uncertainty and the standard deviation of satellite minus TCCON differences is close to unity. Although the exact interpretation of this ratio is difficult, it needs to be determined and reported.

Mean bias:
Computed as the mean difference of satellite minus TCCON retrievals. See also document PVIRv5 (Buchwitz et al., 2017) for an assessment of this quantity using the pre-cursor products.

“Relative systematic error” (or “relative accuracy” or “relative bias” or simply “accuracy”):
To estimate this quantity two values and a combined value are computed and reported:

- The first number is the “spatial bias” computed as standard deviation of the biases as obtained at the various individual TCCON sites. This value is reported in several peer-reviewed publications (e.g., Dils et al., 2014) but does not consider temporal biases (to address this, Dils et al., 2014, computed several quantities: “seasonal mean bias”, “seasonality” and “seasonal relative accuracy”).
- The second number is the “spatio-temporal bias” for a seasonal time scale. There are several options how to compute this number and how to combine it with the first number to get an overall single number for “relative accuracy” and the used method how to exactly compute these numbers has not been fully specified (the most appropriate method may depend on the number of data points, i.e., on the instrument and the applied retrieval algorithm).
- For the QA/QC results presented in this document (and which has been applied to all satellite products discussed in this document) the “spatio-temporal bias”, has been computed as the root-sum-square (RSS) value of the (overall) “spatial bias” and the (overall) “seasonal bias”, i.e., by quadratically adding two numbers.
- The (overall) seasonal bias has been computed as the of the seasonal biases obtained at the individual TCCON sites. The seasonal bias at a given TCCON site has been computed as the standard deviation of the biases in the four (or at least three) seasons. The overall seasonal bias has therefore been computed similarly as the “seasonality” (parameter “Seas”) reported in Dils et al., 2014.
- Because of the used RSS adding method, the “spatio-temporal bias” is always larger than the “spatial bias”. The “spatio-temporal bias” is a positive (or strictly speaking a non-negative) number, and is identified with “relative accuracy” (as it considers spatial and temporal biases).
- However, also other methods are used to compute “spatio-temporal bias” / “relative accuracy”, e.g., by the data provider (DP) method and by the EMMA method.In any case, for the combined value, i.e., for “relative accuracy”, always the larger of the two individual values (“spatial bias” and “spatio-temporal bias”) has been used to report the overall value for “relative accuracy”.

Stability: Linear bias trend (Long term drift):
Computed from the slope as obtained by fitting a straight line to satellite minus TCCON differences using the entire time series. The 1-sigma uncertainty reported is obtained from the slope fit error.

Stability: Year-to-year bias variability:
Computed as maximum minus minimum bias difference of smoothed (using a one year running average) satellite minus TCCON differences.

1.2.1.2.2 Qualitative assessment methods

As the TCCON network is quite sparse it is important for quality assessment of the global satellite-derived data product to also use a number of other (more qualitative) assessment methods.

Therefore, also the following activities have been carried out:

- Generation of global maps and (regional) time series figures to obtain an overview of the entire data set.
- Comparisons with global models (in particular those assimilating accurate surface CO_2 and CH_4 measurements).

1.2.1.3 Methods for comparison of the achieved performance with the user requirements

The results obtained with the "Quantitative assessment methods" are compared with the Target Requirements (TRs) as given in the Target Requirement Document (TRD) (*D4*).

In order to obtain a statement if a certain TR is met or not - or if it is "partially met" - several uncertainties are considered as good as possible:

- The uncertainty of the estimated parameter (e.g., the uncertainties of the obtained values for "accuracy" and "stability").
- The uncertainty of the reference data (here: TCCON) (if not already included in the uncertainty of the obtained values for "accuracy" and "stability").
- The uncertainty of the comparison method (e.g., considering imperfect collocation of the satellite data and the reference data) (if not already included in the uncertainty of the obtained values for "accuracy" and "stability").

The following discussion is limited to "accuracy" and "stability" as these are the most critical / important data quality "figures of merit" and because TRs have been defined for them.

The TRs are the following (see also Target Requirement Document (*TRD, D4*)):

- (Relative) Accuracy XCO_2: < 0.5 ppm (1-sigma)
- Stability XCO_2: < 0.5 ppm/year
- (Relative) Accuracy XCH_4: < 10 ppb (1-sigma)
- Stability XCH_4: < 3 ppb/year

(Relative) Accuracy:

As explained earlier, the term "accuracy" as used here means "relative accuracy" or "relative bias". The reason for this is that a possible "global offset" is not critical for the main application of the data products, which is to use them to obtain information on (regional) sources and sinks. What is critical is the bias difference between different locations and time periods ("spatio-temporal bias"). Nevertheless, the "global offset" (a single number per product) has been determined and is reported in this document (and can be taken into account by the users if needed).

"Accuracy" is essentially estimated from standard deviations of the biases at TCCON validation sites. The estimated value is therefore a positive (strictly speaking a non-negative) number. It is assumed for the following (in line with the description as given in Sect. 1.2.1.2.1) that the value obtained for accuracy has been estimated (for each product and each applied assessment method) assuming error free TCCON observations and an error free comparison method (these errors are considered in a later step).

In order to compute the probability that the accuracy requirement is met, it is required to have at least a rough estimate of the uncertainty ("UNC_ACC") of the reported achieved accuracy value ("ACC"). This uncertainty comes from the uncertainty of the reference data (here TCCON) and the uncertainty of the comparison method (e.g., colocation method and its representativity error).

The uncertainty of the TCCON reference data (see Wunch et al., 2010, but also the discussions of this uncertainty related to the use of TCCON data for the validation of satellite retrievals in Buchwitz et al., 2015, 2016, and Dils et al., 2014) is:

- TCCON uncertainty XCO_2: 0.4 ppm (1-sigma)
- TCCON uncertainty XCH_4: 4 ppb (1-sigma)

These uncertainties are increased by 50% to also consider other error sources, especially error of the comparison method such as the "representativity error". The assumed uncertainty ("UNC_ACC") of the estimated accuracy value ("ACC") are therefore:

- UNC_ACC XCO_2: 0.6 ppm (1-sigma)
- UNC_ACC XCH_4: 6 ppb (1-sigma)

In summary, we now have ACC +/- UNC_ACC (1-sigma) for the estimated relative accuracy or spatio-temporal bias and its uncertainty. These values are interpreted as the mean and the standard deviation of an underlying probability density function (pdf).

ACC is a non-negative number and the Target Requirement (TR) for accuracy defines an "acceptable range" or interval of "acceptable" accuracy values: [0, TR[, i.e., in order to meet the requirements ACC shall be smaller than TR but will be larger than (or equal to) zero. Because of this "non-negativity", ACC cannot be distributed according to a Gaussian ("normal") probability density function (pdf) (esp. if the mean is much smaller than the standard deviation) but it may be reasonable to assume that the overall distribution is a lognormal distribution (https://de.mathworks.com/help/stats/lognormal-distribution.html), with parameters selected such that the lognormal pdf is very similar as a Gaussian pdf if the mean is on the order or larger than the standard deviation.

The probability density function (pdf) of the lognormal distribute is:

$$y = f(x|\mu,\sigma) = \frac{1}{x\sigma\sqrt{2\pi}}\exp\left\{\frac{-(\log x-\mu)^2}{2\sigma^2}\right\}, \quad \text{for } x > 0. \qquad \text{Eq. (1)}$$

The lognormal distribution has parameters μ and σ, which are related to parameters mean m = ACC and variance v = UNC_ACC as follows:

$$\mu = \log\left(m^2/\sqrt{v+m^2}\right) \qquad \text{Eq. (2a)}$$

$$\sigma = \sqrt{\log(v/m^2+1)} \qquad \text{Eq. (2b)}$$

The cumulative distribution function (cdf) of the lognormal distribution is:

$$p = F(x|\mu,\sigma) = \frac{1}{\sigma\sqrt{2\pi}}\int_0^x \frac{1}{t}\exp\left\{\frac{-(\log t-\mu)^2}{2\sigma^2}\right\}dt, \quad \text{for } x > 0. \qquad \text{Eq. (3)}$$

This function is used to compute the probability, that the accuracy requirement is met, see Figure 1 for XCO_2 and Figure 2 for XCH_4.

Figure 1 - Probability that the XCO_2 accuracy TR is met as a function of the achieved accuracy.

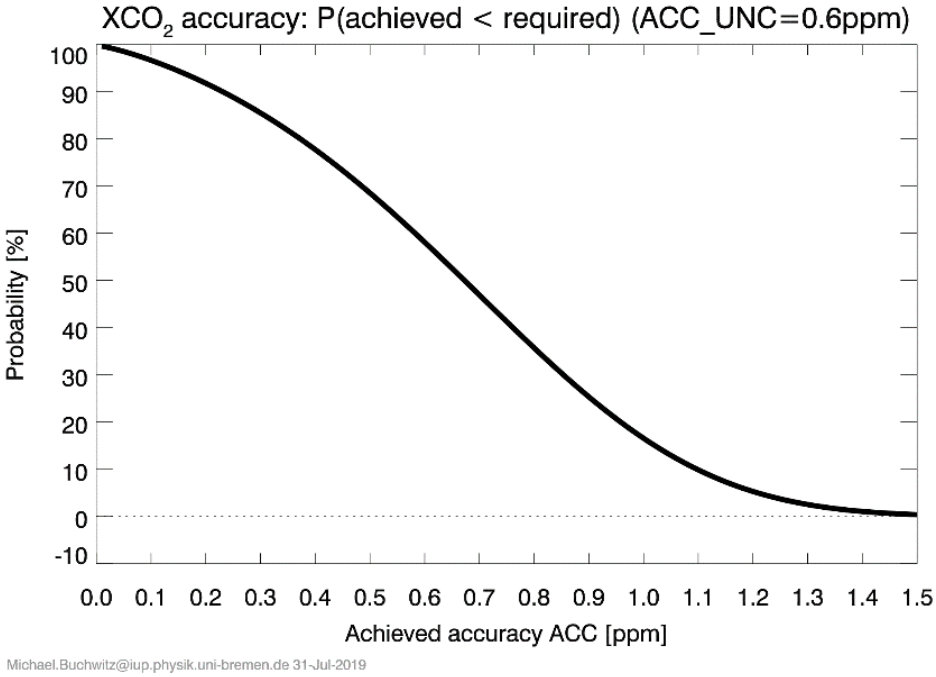
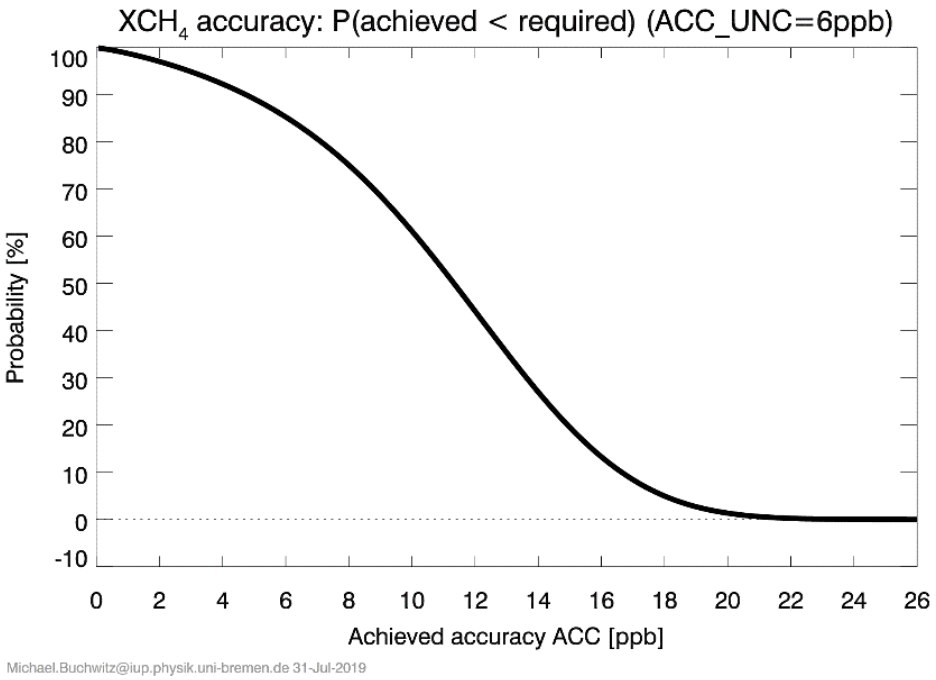


Figure 2 - Probability that the XCH_4 accuracy TR is met as a function of the achieved accuracy.



Stability:

For the TR assessment, the stability assessment is limited to "Linear bias trend / drift" (i.e., the year-to-year bias variability is also determined as explained above but not used for the TR assessment).

As for "accuracy" it is assumed that the value for stability has been obtained assuming error free TCCON observations and an error free comparison method. In contrast to "accuracy" it is assumed that the uncertainty of the stability value is known (it corresponds to the (1-sigma) slope (SLO) error of the linear fit). The result of the stability assessment is: STA +/- UNC_SLO.

To consider the uncertainty of the reference data we assume that the TCCON data approximately meet the following stability requirements:

- XCO_2 stability: 0.2 ppm/year
- XCH_4 stability: 1 ppb/year

These uncertainties need to be added quadratically (via Root-Sum-Square (RSS)) to UNC_SLO to obtain the overall uncertainty UNC_STA.

As shown in Table S-1 for XCO_2 and Table S-2 for XCH_4 in column "Long-term drift" in document PVIRv5 (*Buchwitz et al., 2017*) typical values for STA +/- UNC_SLO are (if the uncertainty is converted to 1-sigma):

- XCO_2: +0.1 +/- 0.07 (1-sigma) ppm/year
- XCH_4: -0.8 +/- 0.4 (1-sigma) ppb/year

These values are listed here only for illustration (the exact value depends on product and assessment method).

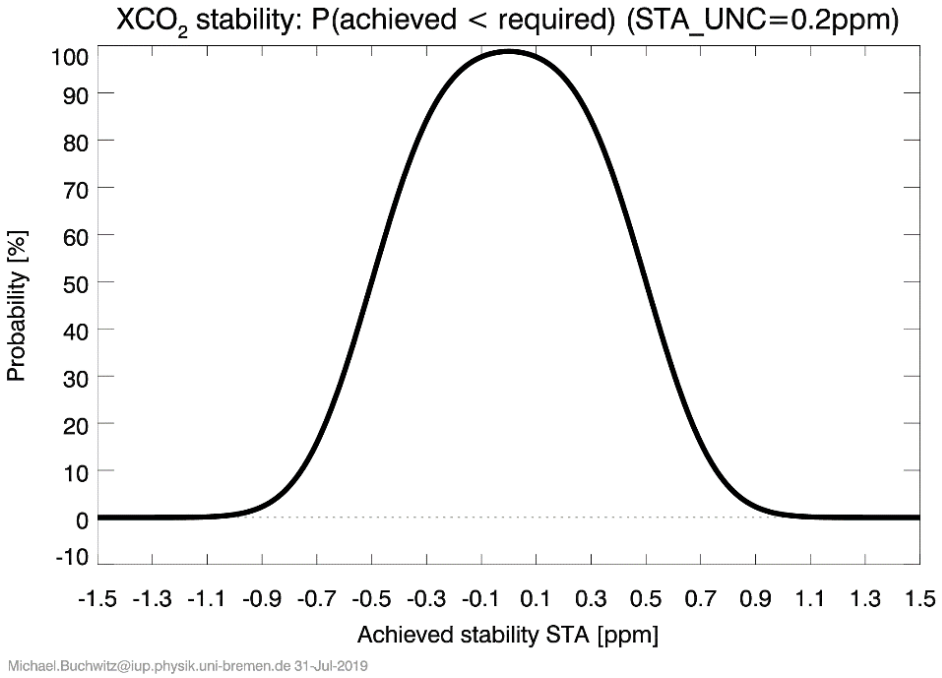
Quadratically adding the assumed TCCON uncertainty gives for this example for STA +/- UNC_STA:

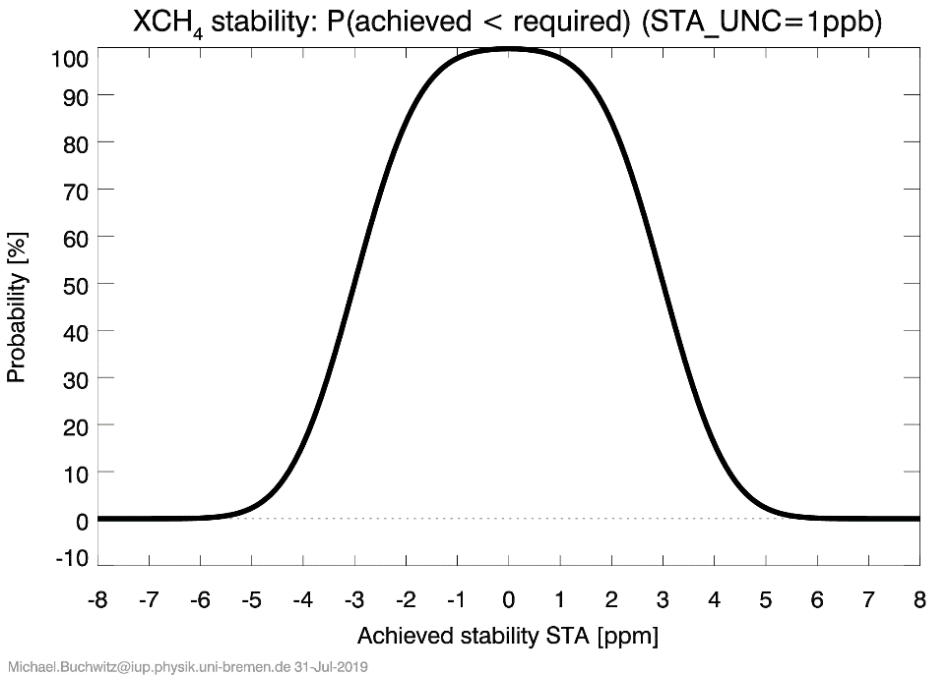
- XCO_2: +0.1 +/- 0.21 (1-sigma) ppm/year
- XCH_4: -0.8 +/- 1.08 (1-sigma) ppb/year

In contrast to ACC, STA can also be negative and we use a Gaussian probability density function N(x, mean=STA, sigma=UNC_STA) to compute the probability that the stability TR is met. This probability is the integral of N over the interval as defined by the stability TR requirement, i.e., interval]-TR, +TR[, or simply the difference between two different values of the cumulative distribution function Nc(x, mean=STA, sigma=UNC_STA) (namely at x=TR and x=-TR). The probability P that the stability TR is met for XCO_2 for a given value of STA is therefore for this example: P(STA) = Nc (+0.5, mean=+0.1, sigma=0.2) – Nc(-0.5, mean=+0.1, sigma=0.2) = 97%. This means that in these cases it is almost certain that the stability TR is met.

Figure 3 shows typical probability functions.

Figure 3 – Probability functions used to obtain the probability that the stability requirement is met. Top: for XCO_2. Bottom: for XCH_4.





1.2.1.4 Known limitations

1.2.1.4.1 TCCON

The TCCON network (https://tccondata.org/) consists of about 25 TCCON sites (see Figure 4). It is relatively dense in the USA, in Europe and in Japan but overall, the TCCON network is relatively sparse (e.g., no or only very few sites in Russia, South America and Africa) and does not cover all conditions, which affect or can affect the quality of the satellite XCO_2 and XCH_4 retrievals (e.g., deserts due to their high surface albedo combined with potentially high amounts of specific aerosol types such as desert dust storm mineral aerosols).

Figure 4 - Location of TCCON sites. Source: https://tccondata.org/.

The TCCON network is the core network for the validation of the satellite XCO_2 and XCH_4 retrievals and is therefore absolutely essential for this part of the C3S service.

It would therefore be highly beneficial for this service

- if the TCCON network were expanded to better cover all geophysical conditions relevant for the quality assessment of the satellite retrievals.
- if the TCCON XCO_2 and XCH_4 retrievals were available faster (current availability: one year after observation).

As a minimum, it needs to be guaranteed that the existing network remains in place but unfortunately even this is currently not guaranteed.

1.2.2 Methods for validation of XCO_2 and XCH_4 Level 3 Obs4MIPs products

The gridded Level 3 XCO_2 and XCH_4 products are in Obs4MIPs format.

The main applications of these products are comparisons with climate models as shown in, e.g., Lauer et al., 2017, presenting a comparison of the version 1 XCO_2 Obs4MIPs data product (see also Reuter et al., 2016). The version 1 XCH_4 Obs4MIPs product is described in Buchwitz et al., 2016a. In February 2017, version 2 of the XCO_2 and XCH_4 Obs4MIPs data products has been generated in the framework of the GHG-CCI project covering the time period 2003-2015 (Buchwitz et al., 2017a; Reuter et al., 2017).

These products have now been re-generated for C3S and they are extended in time (now covering 2003-2016 (version 3)).

The XCO_2 and XCH_4 Obs4MIPs products are based on the XCO_2 and XCH_4 Level 2 products described in this document. The quality of the Obs4MIPs products therefore depends on the quality of the underlying Level 2 products.

Note that the data quality user requirements for the XCO_2 and XCH_4 products (TRD, D4) are requirements for Level 2 products. Explicit data quality requirement for Level 3 products do not exist.

1.2.3 Methods for validation of CO_2 and CH_4 Level 2 mid/upper troposphere products

1.2.3.1 Overview of existing methods as applied to pre-cursor data sets

Past versions of satellite mid/upper tropospheric CO_2 and CH_4 obtained from IASI have been validated using aircraft or, more recently, balloon measurements of atmospheric profiles.

The previous version of the satellite mid/upper tropospheric CO_2 and CH_4 IASI retrievals as generated within the GHG-CCI project of ESA's Climate Change Initiative is called "Climate Research Data Package No. 4" (CRDP4). The quality assessment of this data set is described in the Product Validation and Intercomparison Report, version 5, PVIRv5 (Buchwitz et al., 2017). This GHG-CCI CRDP4 data set is the pre-cursor data set, which has been extended for C3S in the context of the C3S_312a_Lot6 project and its follow-on projects including the current project C3S2_312a_Lot2. As shown in document PVIRv5 (Buchwitz et al., 2017) the validation of the GHG-CCI CRDP4 pre-cursor CO_2 and CH_4 mid/upper tropospheric data products has been carried out by comparison with aircraft and balloon-borne AirCores in-situ profile measurements. These comparisons have been used to validate global trend, growth rate and amplitude of the seasonal cycle. However, due to the scarcity of the measurements, quantity such as single retrieval precision or accuracy remains limited and may be derived only in specific regions where enough measurements are available.

1.2.3.2 Methods applied to the C3S ECV CDR data set

1.2.3.2.1 Quantitative assessment methods

Essentially the same methods have been applied as described in Sect. 1.2.1.2.1 for the XCO_2 and XCH_4 data products, when the number of available aircraft or AirCore measurements of vertical profiles allows the computation of the quantities.

1.2.3.2.2 Qualitative assessment methods

The same methods have been applied as described in Sect. 1.2.1.2.2 for the XCO_2 and XCH_4 data products.

1.2.3.3 Methods for comparison of the achieved performance with the user requirements

Essentially the same methods have been applied as described in Sect. 1.2.1.2.1 for the XCO_2 and XCH_4 data products.

1.2.3.4 Known limitations

The main limitation is the scarcity of measurements in the mid and upper troposphere of CO_2 and CH_4. Moreover, aircraft profiles are generally available up to 6-8 km, which means that the above part of the profile need to be taken from atmospheric transport simulation. This could result in a regional/seasonal bias, which is not well known. Recently developed AirCores, which provide 0-30 km profiles of CO_2 and CH_4 by flying under meteorological balloons, provides a means to fully validate the gas columns retrieved from space, provided that enough measurements are available (less than 20 profiles are currently available worldwide).

For this service, it would thus be highly beneficial:

- if AirCores could be launched regularly at various locations (for instance at existing TCCON/ICOS stations).
- if extensive aircraft campaigns could be organized to collect information in several places where no measurements are currently available (tropical and boreal regions).
- if measurements from IAGOS could include CO_2 and CH_4.

2. Validation results

In this section, detailed validation results are shown. The first two sub-sections present results for validation of the Level 2 XCO_2 (Sect. 2.1) and XCH_4 (Sect. 2.2) data products. The following sub-sections show the validation results for the XCO_2 Level 3 product (Sect. 2.3), for the XCH_4 Level 3 product (Sect. 2.4) and for the Level 2 mid-tropospheric products (Sect. 2.5). In Sect. 4 the results are summarized including comparisons with the user requirements.

For each data product a set of well defined "figures of merit" (FoMs) are computed to summarize the validation results and to compute the probability that the TR is met as explained in Sect. 1.2. This has been done using different approaches depending on, for example, the chosen co-location criteria and other "filters" such as required number of successful co-locations required to "accept" a certain set of FoM (if the number of co-locations is too small than the obtained FoMs may not be regarded as significant or robust enough).

2.1 Validation results for Level 2 XCO_2 products

In this sub-section detailed results from one of the validation approaches for the Level 2 XCO_2 products are presented. This approach is called "QA/QC approach" (see Reuter et al., 2020) and has been developed and used for the validation of all C3S XCO_2 and XCH_4 Level 2 data products.

In addition, also other validation approaches are used, namely the data provider validation approaches (as applied by each data provider to his/her product) and the EMMA approach (see Reuter et al., 2020). These somewhat different approaches are described in the ANNEXes to this Main PQAR document.

This means that an ensemble of validation methods is used to make sure that the overall validation summary results are robust and do not depend on a single method. Note that the same "ensemble approach" for validation has also been used for the GHG-CCI products in the framework of the GHG-CCI project (see Buchwitz et al., 2017).

For the QA/QC method the following so-location criteria have been used:

- Temporal: +/- 2 hours
- Spatial: +/- 2° latitude, +/- 4° longitude

Similar but not necessarily identical criteria have been used for the other validation approaches.

2.1.1 Validation results for product CO2_GOS_OCFP

As a first step, the satellite product is compared with the corresponding TCCON product at each TCCON site separately. Only results from those sites are accepted for further processing if comparisons at least 30 days are possible (note that one day corresponds to one satellite overpass).

Figure 5 shows the comparison at the TCCON site Lamont ("LAM"), Oklahoma, USA. Please see the figure caption for a detailed explanation of the Figures of Merit (FoMs) resulting from this comparison.

As can be seen from Figure 5, also FoMs for seasonal bias and stability are computed. These FoMs are only computed if the time series is "long enough" (at least 3 years) with, for example, a sufficient number of co-locations per season (at least 10 days) and per year (at least 20 days). For Lamont these conditions are fulfilled.

From the results obtained at the individual TCCON sites a single "Product Quality Summary Figure" is produced which is shown as Figure 6 for product CO2_GOS_OCFP. The top right part shows a table listing of the FoMs as obtained for the individual TCCON sites (the Lamont (LAM) results are shown in Figure 5). Listed are

- the TCCON site ID (e.g., LAM_01 for Lamont),
- the random error or single measurement precision (in ppm, 1-sigma),
- the uncertainty ratio "UncR", which is the ratio of the reported XCO_2 uncertainty (as reported in the data product for each individual satellite ground pixel) and the estimated uncertainty as computed from the standard deviation of the difference of the individual observations to TCCON (note that a value not too far away from 1.0 is expected for reliable, i.e., "good quality" reported uncertainties),
- the bias in terms of mean bias and seasonal bias (see Figure 5) and
- FoMs characterising stability in terms of drift and year-to-year bias variability (see caption Figure 5 for details).

The FoMs obtained from the individual sites are used to compute "overall quality FoMs" listed directly below the table of the individual TCCON site results. These overall quality FoMs are obtained by computing (i) the "Mean" and (ii) the standard deviation ("StdDev").

A subset of these FoMs is used to report the final FoMs for the CO2_GOS_OCFP product, which are listed in the yellow marked box in the bottom right of Figure 6:

- Single measurement precision (1-sigma)
- Uncertainty ratio ("UncR")
- Relative accuracy computed as standard deviation of the site-to-site biases as a measure of "regional bias" and also as seasonal bias to include a time dependence
- The global offset or mean bias
- The linear drift component of stability and its 1-sigma uncertainty
- The year-to-year bias component of stability and its 1-sigma uncertainty

Also listed are the probabilities that the accuracy TR and the stability (drift) TR is met (see Sect. 1.2.1.3 for details).

These final FoMs are used for Table 3, which summarizes the quality assessment results for this product.

For the abbreviations of the various TCCON sites as used in Figure 6 please see detailed information as given in Table 3 of Reuter et al., 2020.

Figure 5 - Comparison of satellite XCO_2 product CO2_GOS_OCFP (red symbols in top panel) with TCCON XCO_2 (semi-transparent grey symbols in top panel appearing black in the time series). Top: Daily satellite and TCCON XCO_2 (the number of days is listed (in blue) as Ndays). Also listed are the following figures of merit (in blue): the systematic error (mean bias satellite single observations minus TCCON), mean value of the single observation random error, the number of satellite observations (Nobs) used for the comparisons, the uncertainty ratio "UncRatio", which is the ratio of the reported uncertainty (1-sigma, per ground pixel) and the estimated uncertainty as computed from satellite minus TCCON differences, and the linear correlation coefficient of the daily averaged data ("R(daily)"). Bottom: Daily differences satellite minus TCCON (red symbols). The blue symbols show the 3-monthly biases. The light green line shows the biases at yearly resolution (obtained by smoothing the daily biases). The dark green line shows the linear trend. The corresponding plot statistics are listed at the bottom (reported as mean value and standard deviation) using the same colours as used for the x-y plot: daily bias (in red), 3-monthly bias and overall seasonal bias (blue), linear trend (dark green) and year-to-year bias variability (light green; here the reported value is the peak-to-peak difference and its estimated uncertainty in ppm/year).

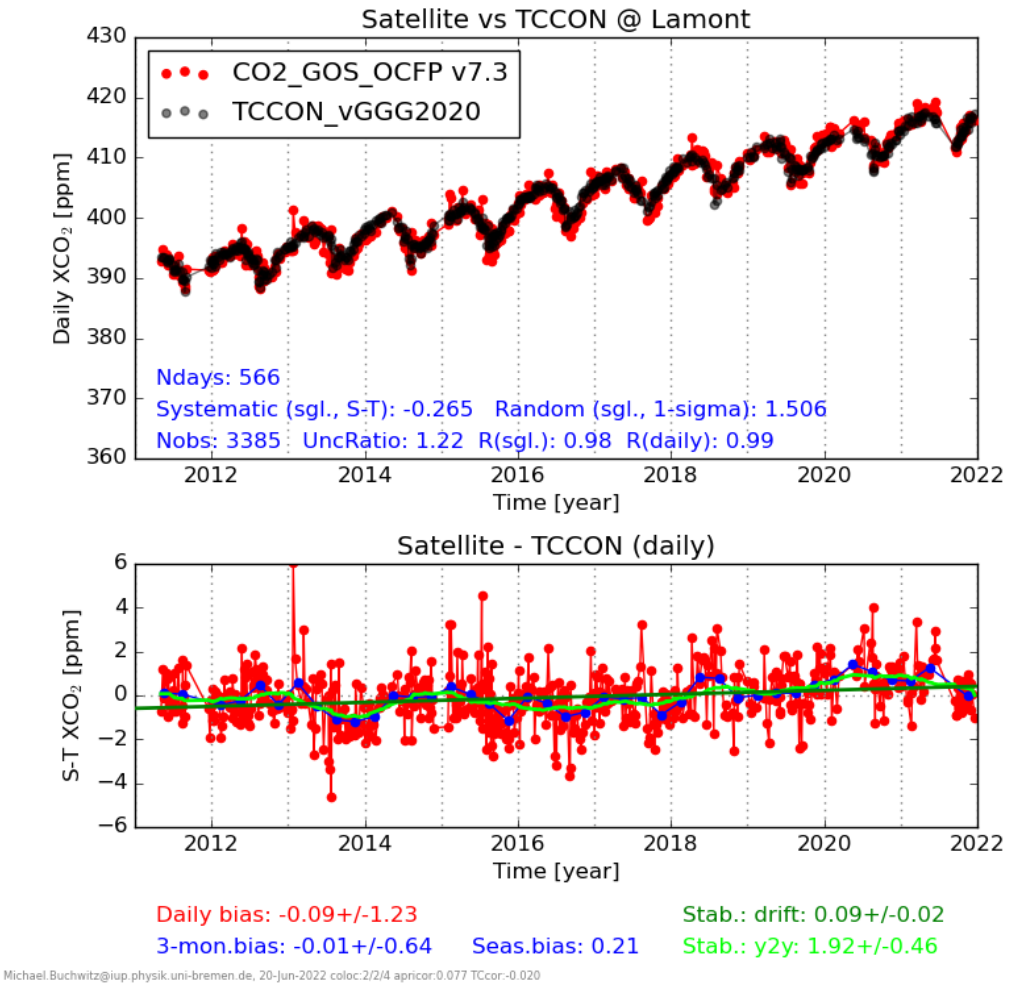
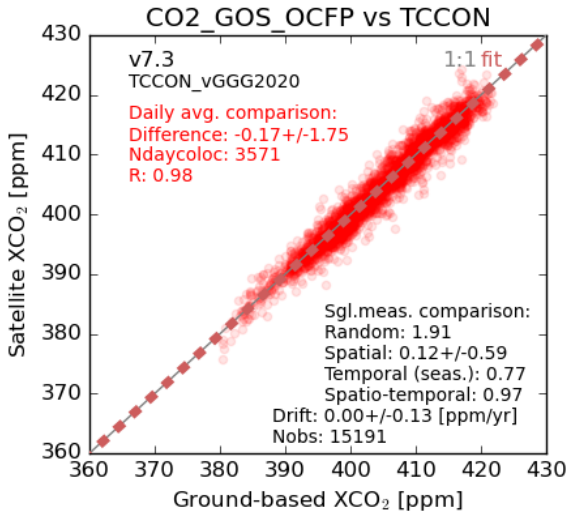
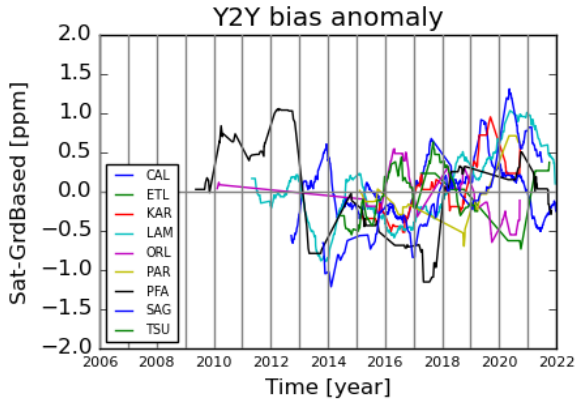


Figure 6 - Product Quality Summary Figure for product CO2_GOS_OCFP. Please see the main text for a detailed explanation. For details on the TCCON sites please see Tab. 3 of Reuter et al., 2020.





Site	Random (sgl.meas.)	UncR	Bias mean	Bias seas	Stability linear drift (+/- 1-sigma)	Stability year-to-year (+/- 1-sigma)
BRE_01	2.06	0.94	0.25		-0.18+/-0.06	
BUR_01	1.77	0.95	0.89		0.41+/-0.18	
CAL_01	2.18	0.82	-0.83	0.51	0.01+/-0.02	1.57+/-0.31
ETL_01	2.01	1.01	0.44		-0.08+/-0.13	1.11+/-0.36
KAR_01	2.16	0.92	0.19	0.64	0.18+/-0.07	1.47+/-0.37
LAM_01	1.51	1.22	-0.27	0.21	0.09+/-0.02	1.92+/-0.46
LAU_02	2.43	0.71	0.85	1.19	-0.22+/-0.13	
LAU_03	2.23	0.72	0.93	1.53	-0.93+/-0.29	
NIC_01	1.39	1.35	-0.15		0.21+/-0.56	
ORL_01	1.79	1.04	-0.04	0.62	-0.02+/-0.04	1.19+/-0.33
PAR_01	2.37	0.77	0.03	1.62	0.08+/-0.10	1.41+/-0.37
PFA_01	1.78	1.13	-0.46	0.37	-0.04+/-0.03	2.21+/-0.62
REU_01	0.98	1.12	0.52		-0.16+/-0.10	
RIK_01	1.89	1.08	-0.58		-0.02+/-0.15	
SAG_01	1.91	1.09	0.43	0.63	0.15+/-0.04	2.52+/-0.57
SOD_01	1.77	1.20	-1.20		-0.27+/-0.20	
TSU_02	1.94	1.12	0.53	0.42	0.04+/-0.06	1.19+/-0.31
XIA_01	2.17	1.00	0.55	0.75	0.76+/-0.20	
Mean	1.91	1.01	0.12	0.77	0.00 0.13	1.62 0.41
StdDev			0.59		0.33	

Sgl.meas.precision (1-sigma): 1.91 UncR: 1.01

Global offset (mean bias): 0.12 (sgl.) / -0.17 (daily)

Relative accuracy: Spat.: 0.59 Seas.: 0.77 Spat.-temp.: 0.97

Stability: Drift (+/- 1-sigma): 0.00 +/- 0.13

Stability: Year-to-year (+/- 1-sigma): 1.62 +/- 0.41

TR accuracy: p(ACC<0.5ppm; 0.97+/-0.60): 18%

TR stability (drift): p(STA:+/-0.5ppm/yr; 0.00+/-0.24): 96%

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Table 3 - Product Quality Summary Table for product CO2_GOS_OCFP as obtained by comparison with TCCON reference data using the QA/QC assessment method. The listed requirements are the threshold (T) requirements as given in *TRD (D4)*. For precision (i.e., single observation statistical uncertainty or random error) also the corresponding breakthrough (B) and goal (G) requirements are listed. For the achieved performance of (relative) "Accuracy" two values are listed: The first one is the spatial component of the bias and the second one is the spatio-temporal bias, computed by also considering seasonal biases. The spatio-temporal bias is our estimate of "relative accuracy". TR refers to "target requirement" and reported is the probability that the corresponding TR is met, i.e., the probabilities that accuracy is better than 0.5 ppm and stability is better than 0.5 ppm/year.

Product Quality Summary Table for Product: CO2_GOS_OCFP Level: 2, Version: 7.3, Time period covered: 4.2009 – 12.2021				
Parameter [unit]	Achieved performance	Requirement	TR	Comments
Single measurement precision (1-sigma) in [ppm]	1.9	< 8 (T) < 3 (B) < 1 (G)	-	-
Uncertainty ratio) in [-]: Ratio reported uncertainty to standard deviation of satellite-TCCON difference	1.01	-	-	No requirement but value close to unity expected for a high quality data product.
Mean bias [ppm]	0.12	-	-	No requirement but value close to zero expected for a high quality data product.
Accuracy: Relative systematic error [ppm]	Spatial – spatiotemporal: 0.59 – 0.97	< 0.5	Probability that accuracy TR is met: 18%	-
Stability: Drift [ppm/year]	0.00 +/- 0.13 (1-sigma)	< 0.5	Probability that stability TR is met: 96%	-
Stability: Year-to-year bias variability [ppm/year]	1.6 +/- 0.4 (1-sigma)	< 0.5	-	-

2.1.2 Validation results for product CO2_GO2_SRFP

Similar figures as shown in Sect. 2.1.1 for product CO2_GOS_OCFP are shown in this section but for product CO2_GOS_SRFP.

The Product Quality Summary Table for product CO2_GOS_SRFP is shown as Table 4.

Figure 7 - As Figure 5 but for product CO2_GOS_SRFP.

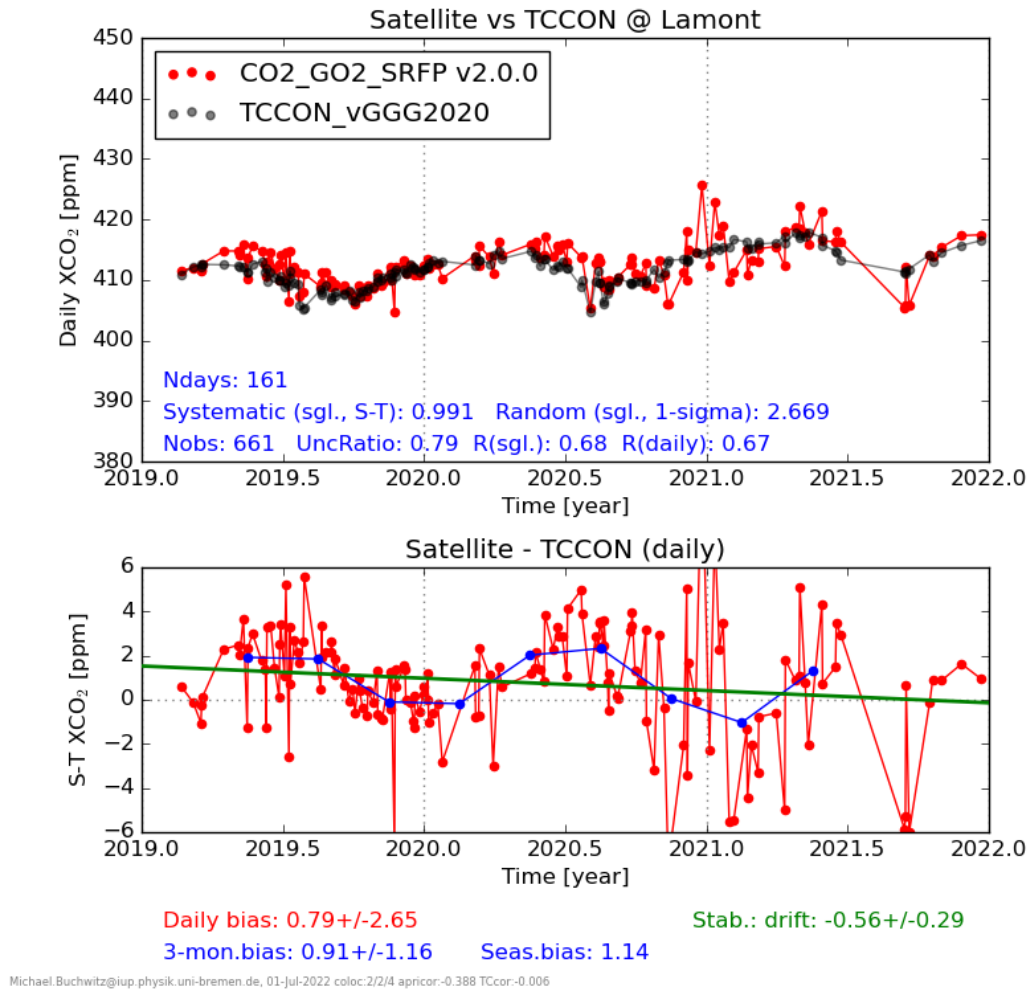
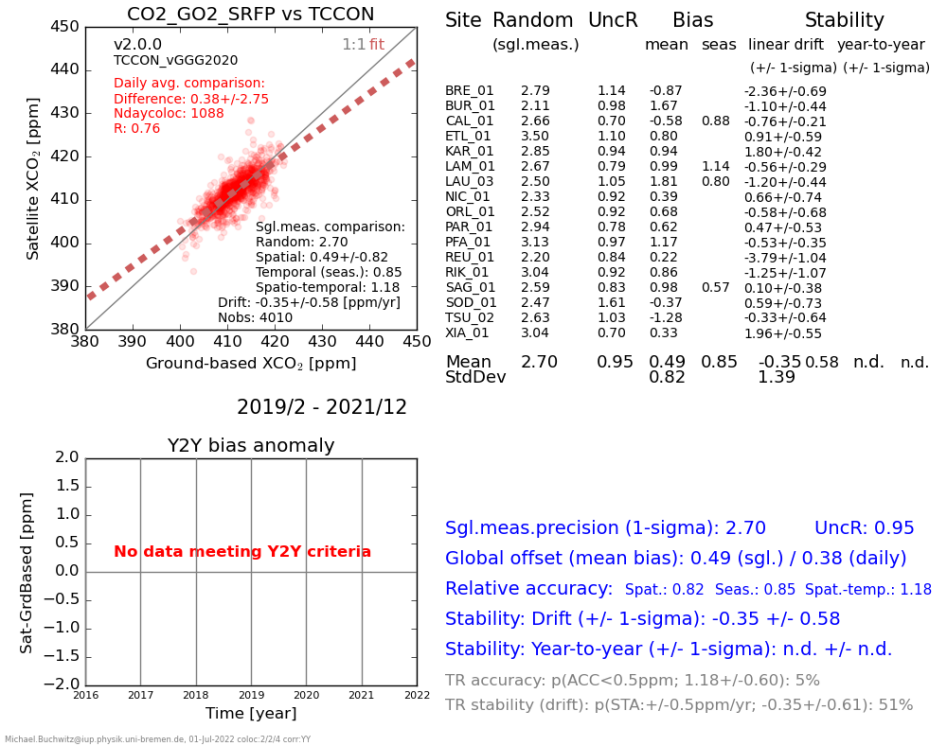


Figure 8 – As Figure 6 but for product CO2_GOS_SRFP.



Site	Random (sgl.meas.)	UncR	Bias mean	Bias seas	Stability linear drift (+/- 1-sigma)	Stability year-to-year (+/- 1-sigma)
BRE_01	2.79	1.14	-0.87		-2.36+/-0.69	
BUR_01	2.11	0.98	1.67		-1.10+/-0.44	
CAL_01	2.66	0.70	-0.58	0.88	-0.76+/-0.21	
ETL_01	3.50	1.10	0.80		0.91+/-0.59	
KAR_01	2.85	0.94	0.94		1.80+/-0.42	
LAM_01	2.67	0.79	0.99	1.14	-0.56+/-0.29	
LAU_03	2.50	1.05	1.81	0.80	-1.20+/-0.44	
NIC_01	2.33	0.92	0.39		0.66+/-0.74	
ORL_01	2.52	0.92	0.68		-0.58+/-0.68	
PAR_01	2.94	0.78	0.62		0.47+/-0.53	
PFA_01	3.13	0.97	1.17		-0.53+/-0.35	
REU_01	2.20	0.84	0.22		-3.79+/-1.04	
RIK_01	3.04	0.92	0.86		-1.25+/-1.07	
SAG_01	2.59	0.83	0.98	0.57	0.10+/-0.38	
SOD_01	2.47	1.61	-0.37		0.59+/-0.73	
TSU_02	2.63	1.03	-1.28		-0.33+/-0.64	
XIA_01	3.04	0.70	0.33		1.96+/-0.55	
Mean	2.70	0.95	0.49	0.85	-0.35	0.58 n.d. n.d.
StdDev			0.82		1.39	

Sgl.meas.precision (1-sigma): 2.70 UncR: 0.95
Global offset (mean bias): 0.49 (sgl.) / 0.38 (daily)
Relative accuracy: Spat.: 0.82 Seas.: 0.85 Spat.-temp.: 1.18
Stability: Drift (+/- 1-sigma): -0.35 +/- 0.58
Stability: Year-to-year (+/- 1-sigma): n.d. +/- n.d.
TR accuracy: p(ACC<0.5ppm; 1.18+/-0.60): 5%
TR stability (drift): p(STA:+/-0.5ppm/yr; -0.35+/-0.61): 51%

Table 4 - Product Quality Summary Table for product CO2_GOS_SRFP. Please see detailed additional info in caption of Table 3.

Product Quality Summary Table for Product: CO2_GO2_SRFP Level: 2, Version: 2.0.0, Time period covered: 02.2019 – 12.2021				
Parameter [unit]	Achieved performance	Requirement	TR	Comments
Single measurement precision (1-sigma) in [ppm]	2.7	< 8 (T) < 3 (B) < 1 (G)	-	-
Uncertainty ratio) in [-]: Ratio reported uncertainty to standard deviation of satellite-TCCON difference	0.95	-	-	No requirement but value close to unity expected for a high quality data product.
Mean bias [ppm]	0.49	-	-	No requirement but value close to zero expected for a high quality data product.
Accuracy: Relative systematic error [ppm]	Spatial – spatiotemporal: 0.82 – 1.18	< 0.5	Probability that accuracy TR is met: 5%	-
Stability: Drift [ppm/year]	-0.35 +/- 0.58 (1-sigma)	< 0.5	Probability that stability TR is met: 51%	-
Stability: Year-to-year bias variability [ppm/year]	Time series too short	< 0.5	-	-

2.1.3 Validation results for product XCO2_EMMA

Similar figures as shown in Sect. 2.1.1 for product CO2_GOS_OCFP are shown in this section but for product XCO2_EMMA.

The Product Quality Summary Table for product XCO2_EMMA is shown as Table 5.

Figure 9 - As Figure 5 but for product XCO2_EMMA.

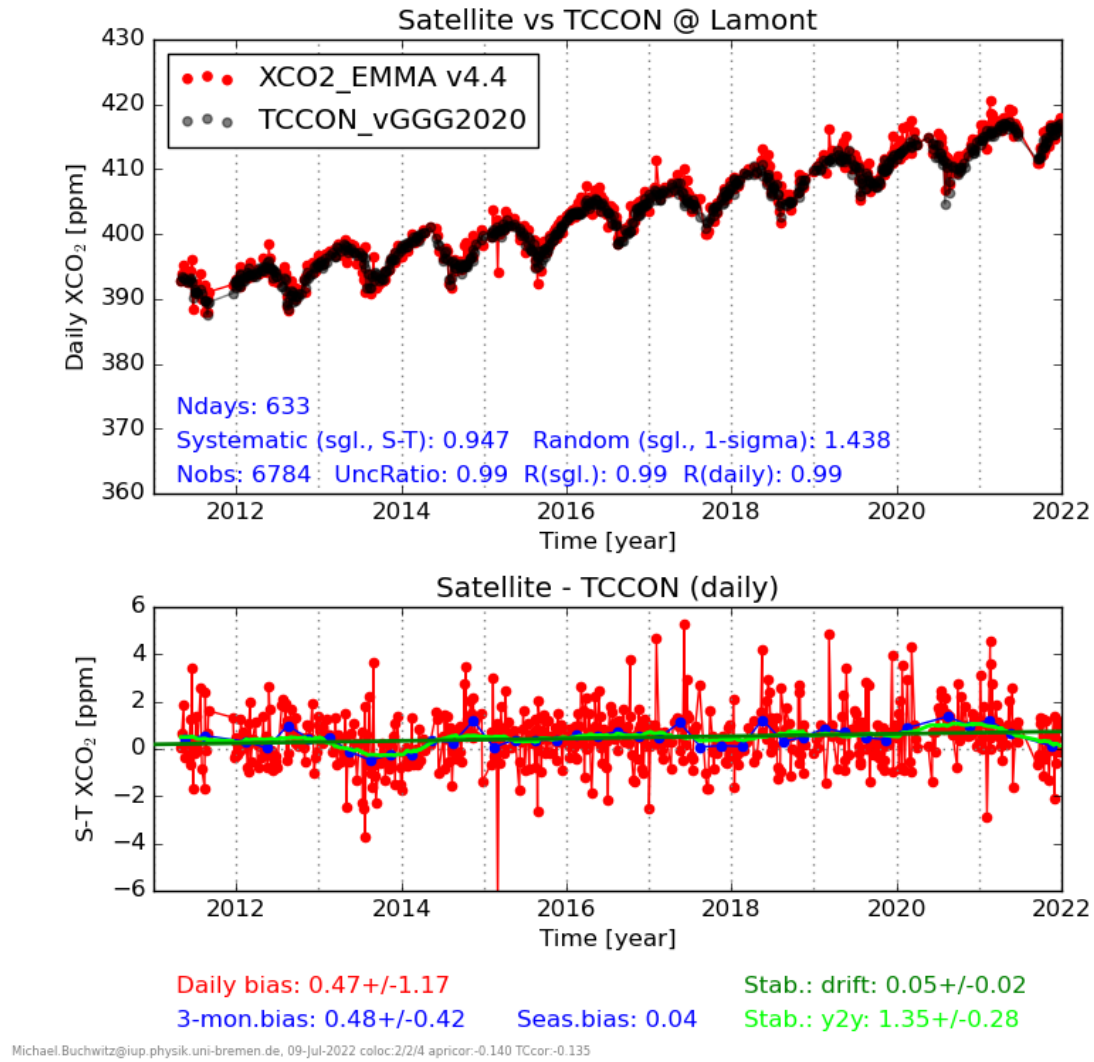
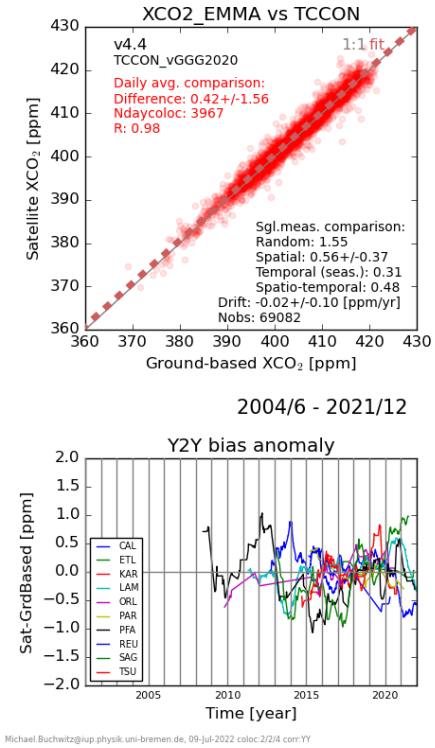


Figure 10 - As Figure 6 but for product XCO2_EMMA.



Site	Random (sgl.meas.)	UncR	Bias mean	Bias seas	Stability linear drift (+/- 1-sigma)	Stability year-to-year (+/- 1-sigma)
BRE_01	1.82	0.97	0.47		-0.08+/-0.05	
BUR_01	1.07	1.30	1.12	0.28	-0.03+/-0.12	
CAL_01	2.08	0.80	-0.27	0.18	-0.09+/-0.02	1.68+/-0.37
ETL_01	1.56	1.10	0.76	0.33	-0.01+/-0.09	0.28+/-0.11
KAR_01	2.10	0.83	0.25	0.47	0.17+/-0.06	1.27+/-0.35
LAM_01	1.44	0.99	0.95	0.04	0.05+/-0.01	1.35+/-0.28
LAU_02	1.31	1.15	0.83	0.02	-0.14+/-0.07	
LAU_03	1.22	0.97	0.65	0.55	-0.34+/-0.22	
NIC_01	1.58	1.02	0.49	0.64	0.41+/-0.40	
ORL_01	1.76	1.02	0.36	0.48	0.07+/-0.03	1.15+/-0.24
PAR_01	1.36	1.16	0.43	0.53	-0.01+/-0.07	0.72+/-0.23
PFA_01	1.57	1.09	0.23	0.31	-0.02+/-0.02	2.11+/-0.50
REU_01	0.95	1.43	0.91	0.18	-0.18+/-0.06	1.12+/-0.33
RIK_01	1.30	1.16	0.58		0.07+/-0.09	
SAG_01	1.25	1.24	0.92	0.08	0.12+/-0.04	1.95+/-0.60
SOD_01	1.58	1.16	-0.14		-1.03+/-0.24	
TSU_02	1.72	1.05	0.47	0.20	0.09+/-0.05	0.93+/-0.17
XIA_01	2.20	0.89	1.01	0.32	0.55+/-0.24	
Mean	1.55	1.07	0.56	0.31	-0.02	0.10 1.25 0.32
StdDev			0.37		0.31	

Sgl.meas.precision (1-sigma): 1.55 UncR: 1.07
Global offset (mean bias): 0.56 (sgl.) / 0.42 (daily)
Relative accuracy: Spat.: 0.37 Seas.: 0.31 Spat.-temp.: 0.48
Stability: Drift (+/- 1-sigma): -0.02 +/- 0.10
Stability: Year-to-year (+/- 1-sigma): 1.25 +/- 0.32
TR accuracy: p(ACC<0.5ppm; 0.48+/-0.60): 69%
TR stability (drift): p(STA:+/-0.5ppm/yr; -0.02+/-0.23): 97%

Table 5 - Product Quality Summary Table for product XCO2_EMMA.

Product Quality Summary Table for Product: XCO2_EMMA Level: 2, Version: 4.4, Time period covered: 01.2003 – 12.2021				
Parameter [unit]	Achieved performance	Requirement	TR	Comments
Single measurement precision (1-sigma) in [ppm]	1.55	< 8 (T) < 3 (B) < 1 (G)	-	-
Uncertainty ratio) in [-]: Ratio reported uncertainty to standard deviation of satellite-TCCON difference	1.07	-	-	No requirement but value close to unity expected for a high quality data product.
Mean bias [ppm]	0.56	-	-	No requirement but value close to zero expected for a high quality data product.
Accuracy: Relative systematic error [ppm]	Spatial – spatiotemporal: 0.37 – 0.48	< 0.5	Probability that accuracy TR is met: 69%	-
Stability: Drift [ppm/year]	-0.02 +/- 0.10 (1-sigma)	< 0.5	Probability that stability TR is met: 97%	-
Stability: Year-to-year bias variability [ppm/year]	1.25 +/- 0.32 (1-sigma)	< 0.5	-	-

2.2 Validation results of Level 2 XCH_4 products

In this sub-section detailed results from one of the validation approaches for the Level 2 XCH_4 products are presented. This approach is called “QA/QC approach” (see Reuter et al., 2020) and has been developed and used for the validation of all C3S XCO_2 and XCH_4 Level 2 data products.

In addition, also other validation approaches are used, namely the data provider validation approaches (as applied by each data provider to his/her product) and the EMMA approach (see Reuter et al., 2020). These somewhat different approaches are described in the ANNEXes to this Main PQAR document.

This means that an ensemble of validation methods is used to make sure that the overall validation summary results are robust and do not depend on a single method. Note that the same “ensemble approach” for validation has also been used for the GHG-CCI products in the framework of the GHG-CCI project (see Buchwitz et al., 2017).

For the QA/QC method the following so-location criteria have been used:

- Temporal: +/- 2 hours
- Spatial: +/- 2° latitude, +/- 4° longitude

Similar but not necessarily identical criteria have been used for the other validation approaches.

2.2.1 Validation results for product CH4_GOS_OCFP

Similar figures as shown in Sect. 2.1.1 for product CO2_GOS_OCFP are shown in this section but for product CH4_GOS_OCFP.

The Product Quality Summary Table for product CH4_GOS_OCFP is shown as Table 6.

Figure 11 - As Figure 5 but for product CH4_GOS_OCFP.

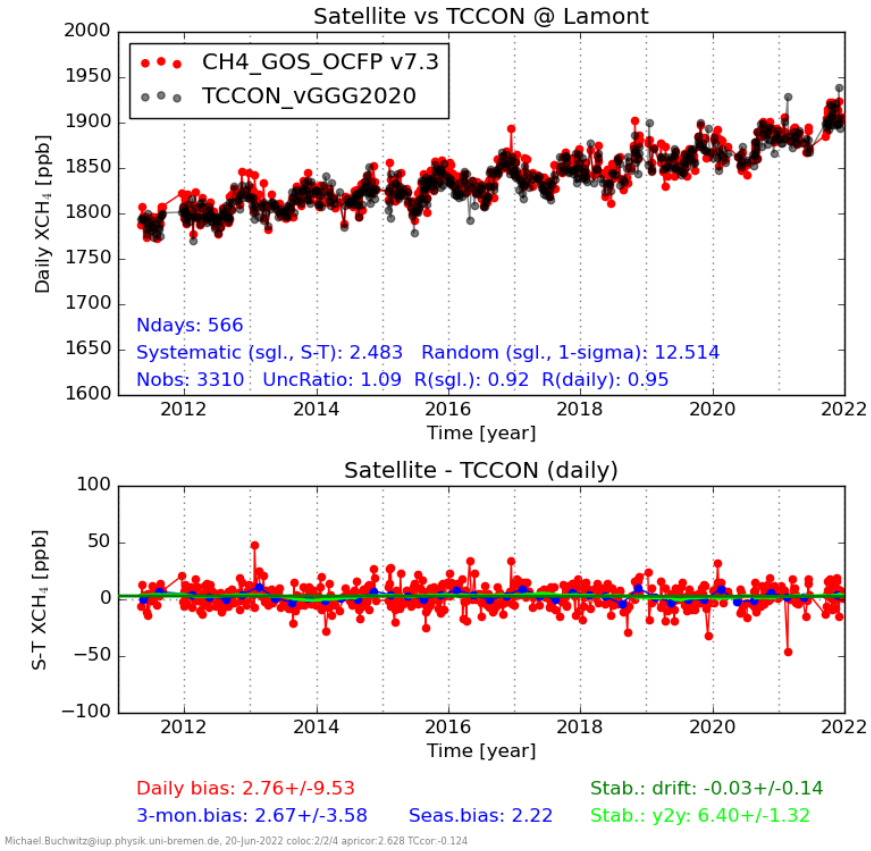
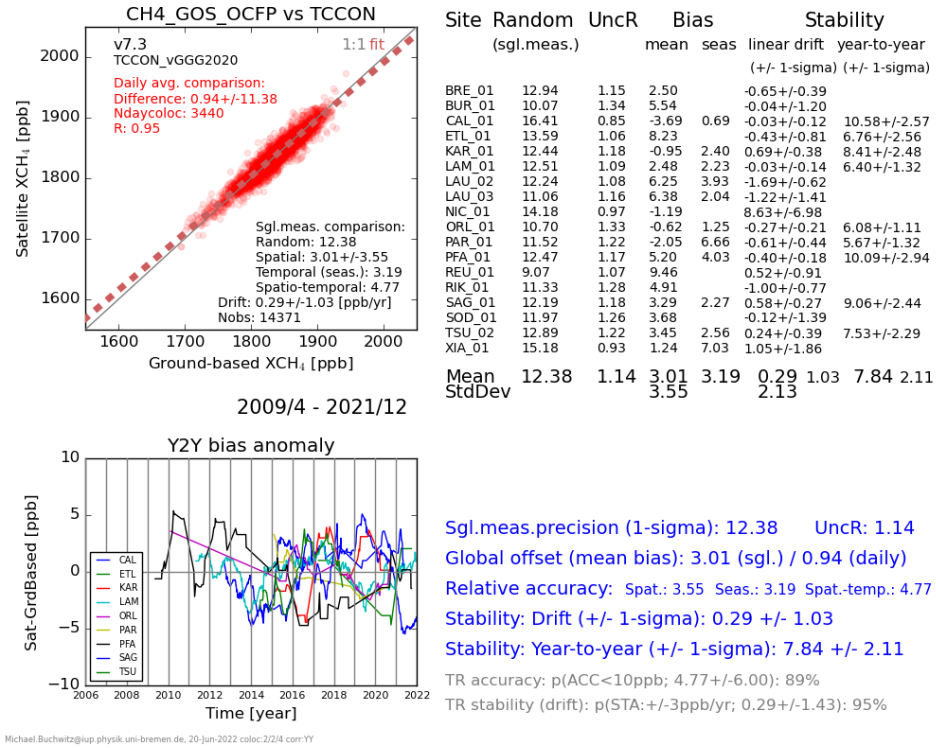


Figure 12 - As Figure 6 but for product CH4_GOS_OCFP.



Site	Random (sgl.meas.)	UncR	Bias mean	Bias seas	Stability linear drift (+/- 1-sigma)	Stability year-to-year (+/- 1-sigma)
BRE_01	12.94	1.15	2.50		-0.65+/-0.39	
BUR_01	10.07	1.34	5.54		-0.04+/-1.20	
CAL_01	16.41	0.85	-3.69	0.69	-0.03+/-0.12	10.58+/-2.57
ETL_01	13.59	1.06	8.23		-0.43+/-0.81	6.76+/-2.56
KAR_01	12.44	1.18	-0.95	2.40	0.69+/-0.38	8.41+/-2.48
LAM_01	12.51	1.09	2.48	2.23	-0.03+/-0.14	6.40+/-1.32
LAU_02	12.24	1.08	6.25	3.93	-1.69+/-0.62	
LAU_03	11.06	1.16	6.38	2.04	-1.22+/-1.41	
NIC_01	14.18	0.97	-1.19		8.63+/-6.98	
ORL_01	10.70	1.33	-0.62	1.25	-0.27+/-0.21	6.08+/-1.11
PAR_01	11.52	1.22	-2.05	6.66	-0.61+/-0.44	5.67+/-1.32
PFA_01	12.47	1.17	5.20	4.03	-0.40+/-0.18	10.09+/-2.94
REU_01	9.07	1.07	9.46		0.52+/-0.91	
RIK_01	11.33	1.28	4.91		-1.00+/-0.77	
SAG_01	12.19	1.18	3.29	2.27	0.58+/-0.27	9.06+/-2.44
SOD_01	11.97	1.26	3.68		-0.12+/-1.39	
TSU_02	12.89	1.22	3.45	2.56	0.24+/-0.39	7.53+/-2.29
XIA_01	15.18	0.93	1.24	7.03	1.05+/-1.86	
Mean	12.38	1.14	3.01	3.19	0.29 1.03	7.84 2.11
StdDev			3.55		2.13	

Sgl.meas.precision (1-sigma): 12.38 UncR: 1.14
Global offset (mean bias): 3.01 (sgl.) / 0.94 (daily)
Relative accuracy: Spat.: 3.55 Seas.: 3.19 Spat.-temp.: 4.77
Stability: Drift (+/- 1-sigma): 0.29 +/- 1.03
Stability: Year-to-year (+/- 1-sigma): 7.84 +/- 2.11
TR accuracy: p(ACC<10ppb; 4.77+/-6.00): 89%
TR stability (drift): p(STA:+/-3ppb/yr; 0.29+/-1.43): 95%

Table 6 - Product Quality Summary Table for product CH4_GOS_OCFP.

Product Quality Summary Table for Product: CH4_GOS_OCFP Level: 2, Version: 7.3, Time period covered: 04.2009 – 12.2021				
Parameter [unit]	Achieved performance	Requirement	TR	Comments
Single measurement precision (1-sigma) in [ppb]	12.4	< 34 (T) < 17 (B) < 9 (G)	-	-
Uncertainty ratio) in [-]: Ratio reported uncertainty to standard deviation of satellite-TCCON difference	1.14	-	-	No requirement but value close to unity expected for a high quality data product.
Mean bias [ppb]	3.0	-	-	No requirement but value close to zero expected for a high quality data product.
Accuracy: Relative systematic error [ppb]	Spatial – spatiotemporal: 3.6 – 4.8	< 10	Probability that accuracy TR is met: 89%	-
Stability: Linear bias trend [ppb/year]	0.3 +/- 1.0 (1-sigma)	< 3	Probability that stability TR is met: 95%	-
Stability: Year-to-year bias variability [ppb/year]	8 +/- 2 (1-sigma)	< 3	-	-

2.2.2 Validation results for product CH4_GOS_OCPR

Similar figures as shown in Sect. 2.1.1 for product CO2_GOS_OCFP are shown in this section but for product CH4_GOS_OCPR.

The Product Quality Summary Table for product CH4_GOS_OCPR is shown as Table 7.

Figure 13 - As Figure 5 but for product CH4_GOS_OCPR.

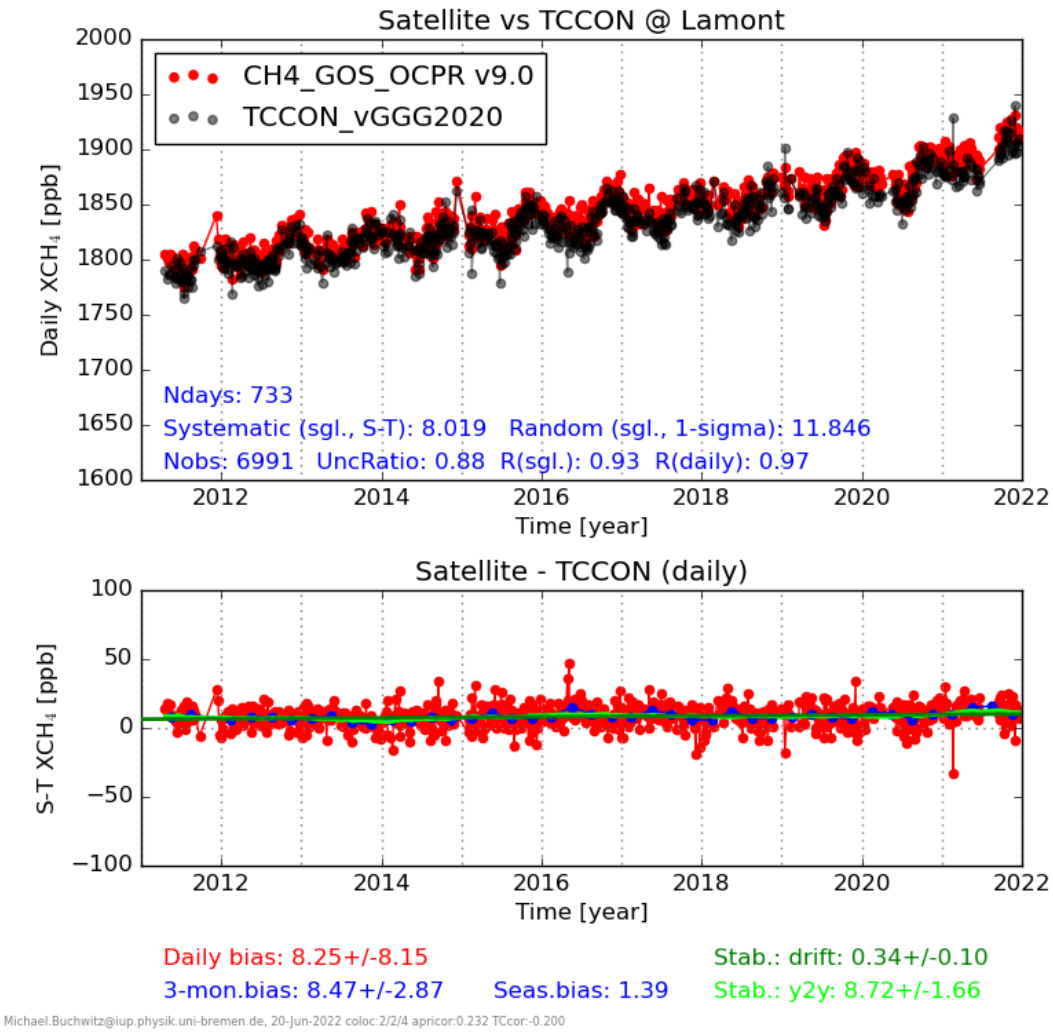
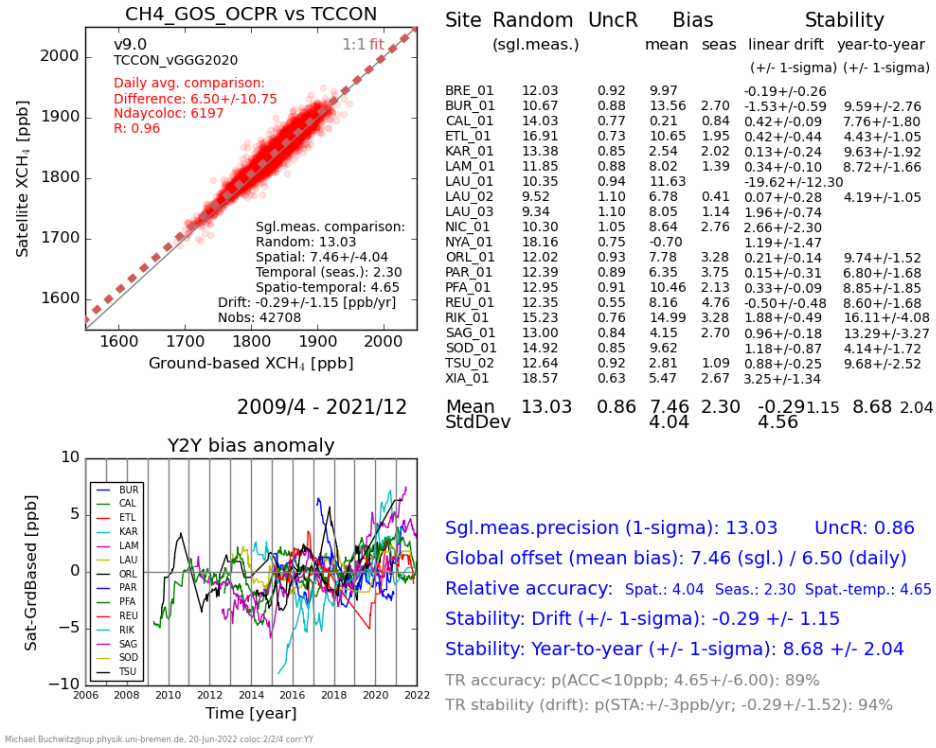


Figure 14 - As Figure 6 but for product CH4_GOS_OCPR.



Site	Random (sgl.meas.)	UncR	Bias mean	Bias seas	Stability linear drift (+/- 1-sigma)	Stability year-to-year (+/- 1-sigma)
BRE_01	12.03	0.92	9.97		-0.19+/-0.26	
BUR_01	10.67	0.88	13.56	2.70	-1.53+/-0.59	9.59+/-2.76
CAL_01	14.03	0.77	0.21	0.84	0.42+/-0.09	7.76+/-1.80
ETL_01	16.91	0.73	10.65	1.95	0.42+/-0.44	4.43+/-1.05
KAR_01	13.38	0.85	2.54	2.02	0.13+/-0.24	9.63+/-1.92
LAM_01	11.85	0.88	8.02	1.39	0.34+/-0.10	8.72+/-1.66
LAU_01	10.35	0.94	11.63		-19.62+/-12.30	
LAU_02	9.52	1.10	6.78	0.41	0.07+/-0.28	4.19+/-1.05
LAU_03	9.34	1.10	8.05	1.14	1.96+/-0.74	
NIC_01	10.30	1.05	8.64	2.76	2.66+/-2.30	
NYA_01	18.16	0.75	-0.70		1.19+/-1.47	
ORL_01	12.02	0.93	7.78	3.28	0.21+/-0.14	9.74+/-1.52
PAR_01	12.39	0.89	6.35	3.75	0.15+/-0.31	6.80+/-1.68
PFA_01	12.95	0.91	10.46	2.13	0.33+/-0.09	8.85+/-1.85
REU_01	12.35	0.55	8.16	4.76	-0.50+/-0.48	8.60+/-1.68
RIK_01	15.23	0.76	14.99	3.28	1.88+/-0.49	16.11+/-4.08
SAG_01	13.00	0.84	4.15	2.70	0.96+/-0.18	13.29+/-3.27
SOD_01	14.92	0.85	9.62		1.18+/-0.87	4.14+/-1.72
TSU_02	12.64	0.92	2.81	1.09	0.88+/-0.25	9.68+/-2.52
XIA_01	18.57	0.63	5.47	2.67	3.25+/-1.34	
Mean	13.03	0.86	7.46	2.30	-0.29	8.68
StdDev			4.04		1.15 4.56	2.04

Sgl.meas.precision (1-sigma): 13.03 UncR: 0.86
Global offset (mean bias): 7.46 (sgl.) / 6.50 (daily)
Relative accuracy: Spat.: 4.04 Seas.: 2.30 Spat.-temp.: 4.65
Stability: Drift (+/- 1-sigma): -0.29 +/- 1.15
Stability: Year-to-year (+/- 1-sigma): 8.68 +/- 2.04
TR accuracy: p(ACC<10ppb; 4.65+/-6.00): 89%
TR stability (drift): p(STA:+/-3ppb/yr; -0.29+/-1.52): 94%

Table 7 - Product Quality Summary Table for product CH4_GOS_OCPR.

Product Quality Summary Table for Product: CH4_GOS_OCPR Level: 2, Version: 9.0, Time period covered: 4.2009 – 12.2021				
Parameter [unit]	Achieved performance	Requirement	TR	Comments
Single measurement precision (1-sigma) in [ppb]	13	< 34 (T) < 17 (B) < 9 (G)	-	-
Uncertainty ratio) in [-]: Ratio reported uncertainty to standard deviation of satellite-TCCON difference	0.86	-	-	No requirement but value close to unity expected for a high quality data product.
Mean bias [ppb]	4.0	-	-	No requirement but value close to zero expected for a high quality data product.
Accuracy: Relative systematic error [ppb]	Spatial – spatiotemporal: 4.0 – 4.7	< 10	Probability that accuracy TR is met: 89%	-
Stability: Linear bias trend [ppb/year]	-0.3 +/- 1.2 (1-sigma)	< 3	Probability that stability TR is met: 94%	-
Stability: Year-to-year bias variability [ppb/year]	9 +/- 2 (1-sigma)	< 3	-	-

2.2.3 Validation results for product CH4_GO2_SRFP

Similar figures as shown in Sect. 2.1.1 for product CO2_GOS_OCFP are shown in this section but for product CH4_GO2_SRFP.

The Product Quality Summary Table for product CH4_GO2_SRFP is shown as Table 8.

Figure 15 - As Figure 5 but for product CH4_GO2_SRFP.

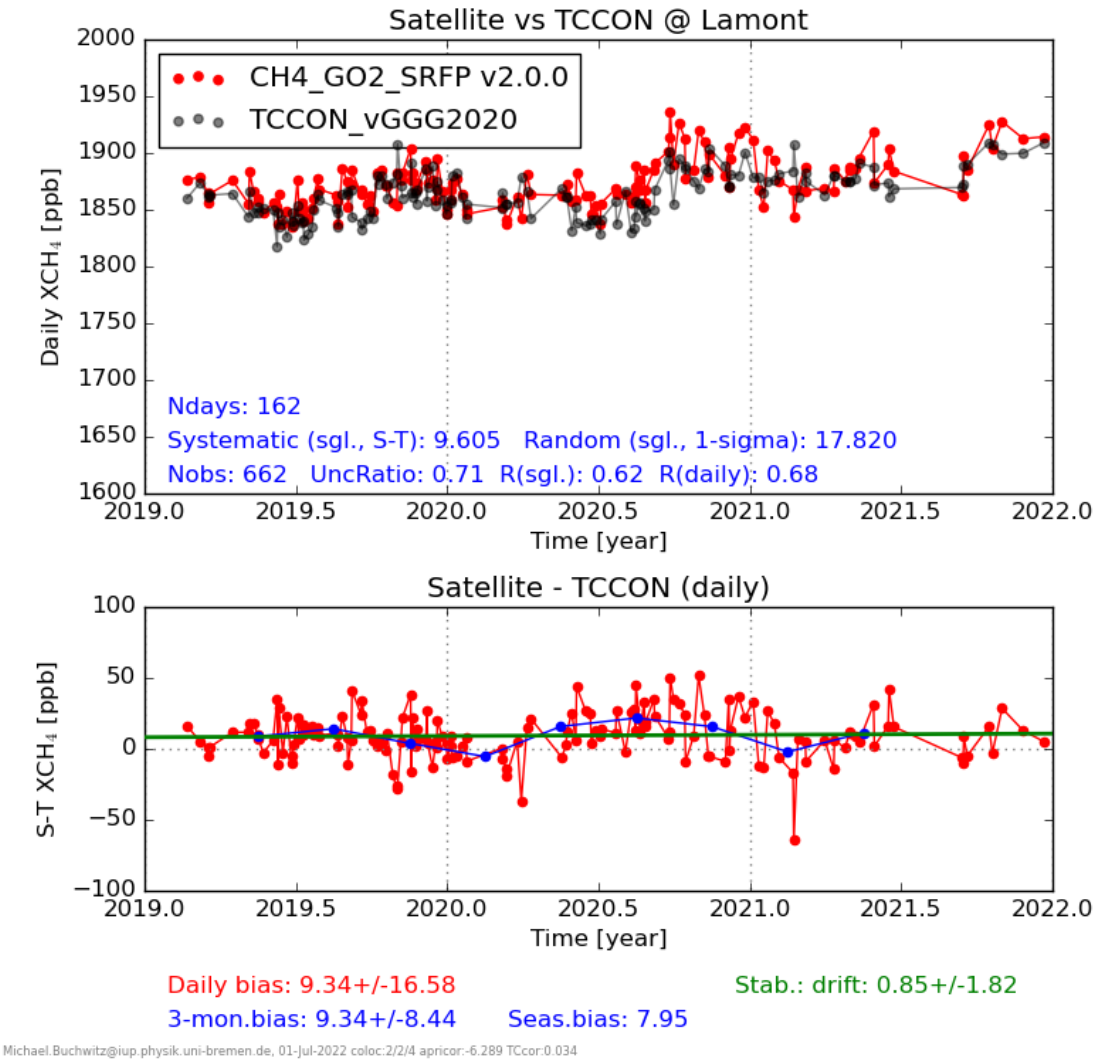
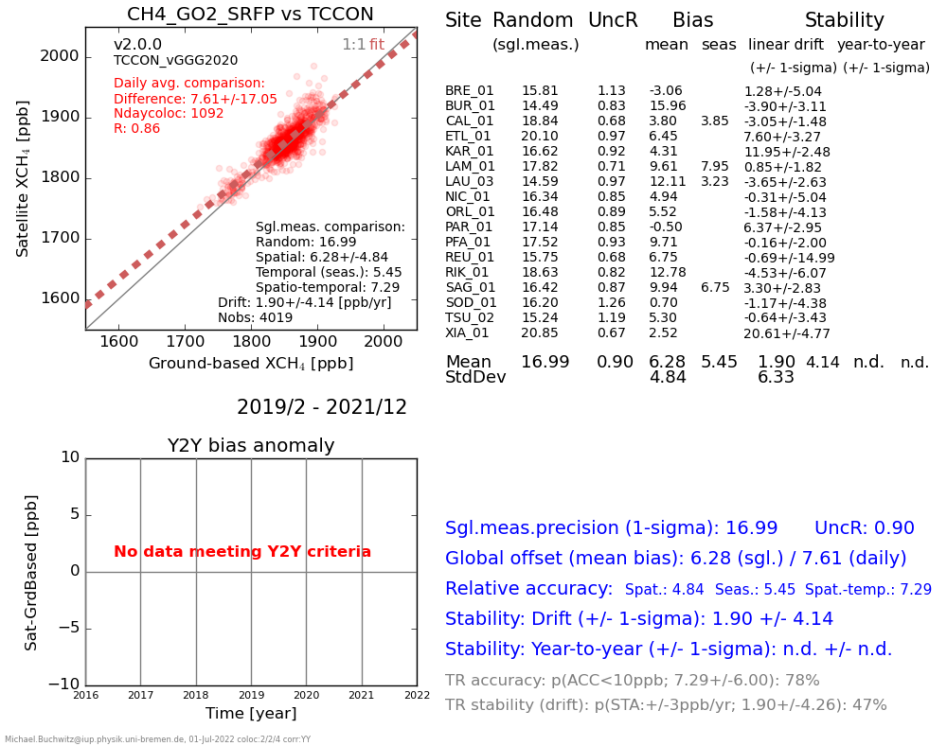


Figure 16 - As Figure 6 but for product CH4_GO2_SRFP.



Site	Random (sgl.meas.)	UncR	Bias mean	Bias seas	Stability linear drift (+/- 1-sigma)	Stability year-to-year (+/- 1-sigma)		
BRE_01	15.81	1.13	-3.06		1.28+/-5.04			
BUR_01	14.49	0.83	15.96		-3.90+/-3.11			
CAL_01	18.84	0.68	3.80	3.85	-3.05+/-1.48			
ETL_01	20.10	0.97	6.45		7.60+/-3.27			
KAR_01	16.62	0.92	4.31		11.95+/-2.48			
LAM_01	17.82	0.71	9.61	7.95	0.85+/-1.82			
LAU_03	14.59	0.97	12.11	3.23	-3.65+/-2.63			
NIC_01	16.34	0.85	4.94		-0.31+/-5.04			
ORL_01	16.48	0.89	5.52		-1.58+/-4.13			
PAR_01	17.14	0.85	-0.50		6.37+/-2.95			
PFA_01	17.52	0.93	9.71		-0.16+/-2.00			
REU_01	15.75	0.68	6.75		-0.69+/-14.99			
RIK_01	18.63	0.82	12.78		-4.53+/-6.07			
SAG_01	16.42	0.87	9.94	6.75	3.30+/-2.83			
SOD_01	16.20	1.26	0.70		-1.17+/-4.38			
TSU_02	15.24	1.19	5.30		-0.64+/-3.43			
XIA_01	20.85	0.67	2.52		20.61+/-4.77			
Mean	16.99	0.90	6.28	5.45	1.90	4.14	n.d.	n.d.
StdDev			4.84		6.33			

Sgl.meas.precision (1-sigma): 16.99 UncR: 0.90
Global offset (mean bias): 6.28 (sgl.) / 7.61 (daily)
Relative accuracy: Spat.: 4.84 Seas.: 5.45 Spat.-temp.: 7.29
Stability: Drift (+/- 1-sigma): 1.90 +/- 4.14
Stability: Year-to-year (+/- 1-sigma): n.d. +/- n.d.
TR accuracy: p(ACC<10ppb; 7.29+/-6.00): 78%
TR stability (drift): p(STA:+/-3ppb/yr; 1.90+/-4.26): 47%

Table 8 - Product Quality Summary Table for product CH4_GO2_SRFP.

Product Quality Summary Table for Product: CH4_GO2_SRFP Level: 2, Version: 2.0.0, Time period covered: 02.2019 – 12.2021				
Parameter [unit]	Achieved performance	Requirement	TR	Comments
Single measurement precision (1-sigma) in [ppb]	17.0	< 34 (T) < 17 (B) < 9 (G)	-	-
Uncertainty ratio) in [-]: Ratio reported uncertainty to standard deviation of satellite-TCCON difference	0.90	-	-	No requirement but value close to unity expected for a high quality data product.
Mean bias [ppb]	6.3	-	-	No requirement but value close to zero expected for a high quality data product.
Accuracy: Relative systematic error [ppb]	Spatial – spatiotemporal: 4.8 – 7.3	< 10	Probability that accuracy TR is met: 78%	-
Stability: Linear bias trend [ppb/year]	1.9 +/- 4.1 (1-sigma)	< 3	Probability that stability TR is met: 47%	-
Stability: Year-to-year bias variability [ppb/year]	Time series too short	< 3	-	-

2.2.4 Validation results for product CH4_GO2_SRPR

Similar figures as shown in Sect. 2.1.1 for product CO2_GOS_OCFP are shown in this section but for product CH4_GO2_SRPR.

The Product Quality Summary Table for product CH4_GO2_SRPR is shown as Table 9.

Figure 17 - As Figure 5 but for product CH4_GO2_SRPR.

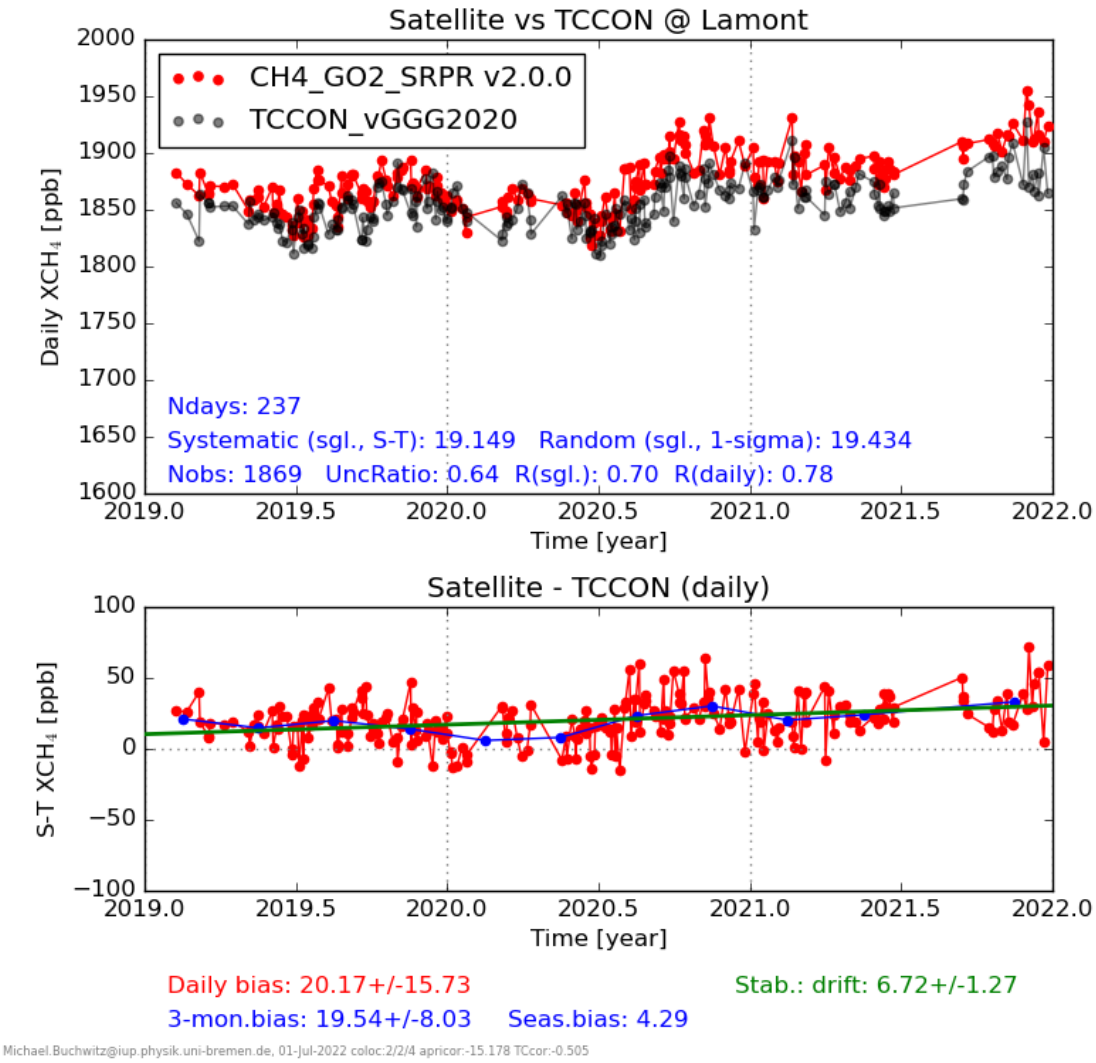
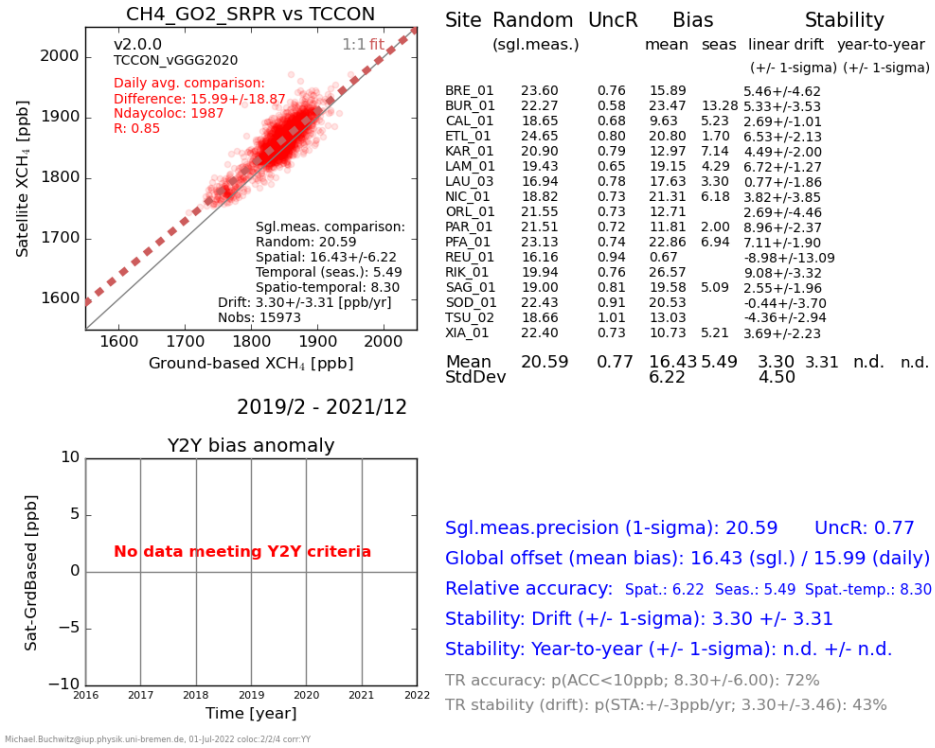


Figure 18 – As Figure 6 but for product CH4_GO2_SRPR.



Site	Random (sgl.meas.)	UncR	Bias mean	Bias seas	Stability linear drift (+/- 1-sigma)	Stability year-to-year (+/- 1-sigma)
BRE_01	23.60	0.76	15.89		5.46+/-4.62	
BUR_01	22.27	0.58	23.47	13.28	5.33+/-3.53	
CAL_01	18.65	0.68	9.63	5.23	2.69+/-1.01	
ETL_01	24.65	0.80	20.80	1.70	6.53+/-2.13	
KAR_01	20.90	0.79	12.97	7.14	4.49+/-2.00	
LAM_01	19.43	0.65	19.15	4.29	6.72+/-1.27	
LAU_03	16.94	0.78	17.63	3.30	0.77+/-1.86	
NIC_01	18.82	0.73	21.31	6.18	3.82+/-3.85	
ORL_01	21.55	0.73	12.71		2.69+/-4.46	
PAR_01	21.51	0.72	11.81	2.00	8.96+/-2.37	
PFA_01	23.13	0.74	22.86	6.94	7.11+/-1.90	
REU_01	16.16	0.94	0.67		-8.98+/-13.09	
RIK_01	19.94	0.76	26.57		9.08+/-3.32	
SAG_01	19.00	0.81	19.58	5.09	2.55+/-1.96	
SOD_01	22.43	0.91	20.53		-0.44+/-3.70	
TSU_02	18.66	1.01	13.03		-4.36+/-2.94	
XIA_01	22.40	0.73	10.73	5.21	3.69+/-2.23	
Mean	20.59	0.77	16.43	5.49	3.30	3.31 n.d. n.d.
StdDev			6.22		4.50	

Sgl.meas.precision (1-sigma): 20.59 UncR: 0.77
Global offset (mean bias): 16.43 (sgl.) / 15.99 (daily)
Relative accuracy: Spat.: 6.22 Seas.: 5.49 Spat.-temp.: 8.30
Stability: Drift (+/- 1-sigma): 3.30 +/- 3.31
Stability: Year-to-year (+/- 1-sigma): n.d. +/- n.d.
TR accuracy: p(ACC<10ppb; 8.30+/-6.00): 72%
TR stability (drift): p(STA:+/-3ppb/yr; 3.30+/-3.46): 43%

Table 9 - Product Quality Summary Table for product CH4_GO2_SRPR.

Product Quality Summary Table for Product: CH4_GO2_SRPR Level: 2, Version: 2.0.0, Time period covered: 02.2019 – 12.2021				
Parameter [unit]	Achieved performance	Requirement	TR	Comments
Single measurement precision (1-sigma) in [ppb]	20.6	< 34 (T) < 17 (B) < 9 (G)	-	-
Uncertainty ratio) in [-]: Ratio reported uncertainty to standard deviation of satellite-TCCON difference	0.77	-	-	No requirement but value close to unity expected for a high quality data product.
Mean bias [ppb]	16.4	-	-	No requirement but value close to zero expected for a high quality data product.
Accuracy: Relative systematic error [ppb]	Spatial – spatiotemporal: 6.2 – 8.3	< 10	Probability that accuracy TR is met: 72%	-
Stability: Linear bias trend [ppb/year]	3.3 +/- 3.3 (1-sigma)	< 3	Probability that stability TR is met: 43%	-
Stability: Year-to-year bias variability [ppb/year]	Time series too short	< 3	-	-

2.2.5 Validation results for product XCH4_EMMA

Similar figures as shown in Sect. 2.1.1 for product CO2_GOS_OCFP are shown in this section but for product XCH4_EMMA.

The Product Quality Summary Table for product XCH4_EMMA is shown as Table 10.

Figure 19 - As Figure 5 but for product XCH4_EMMA.

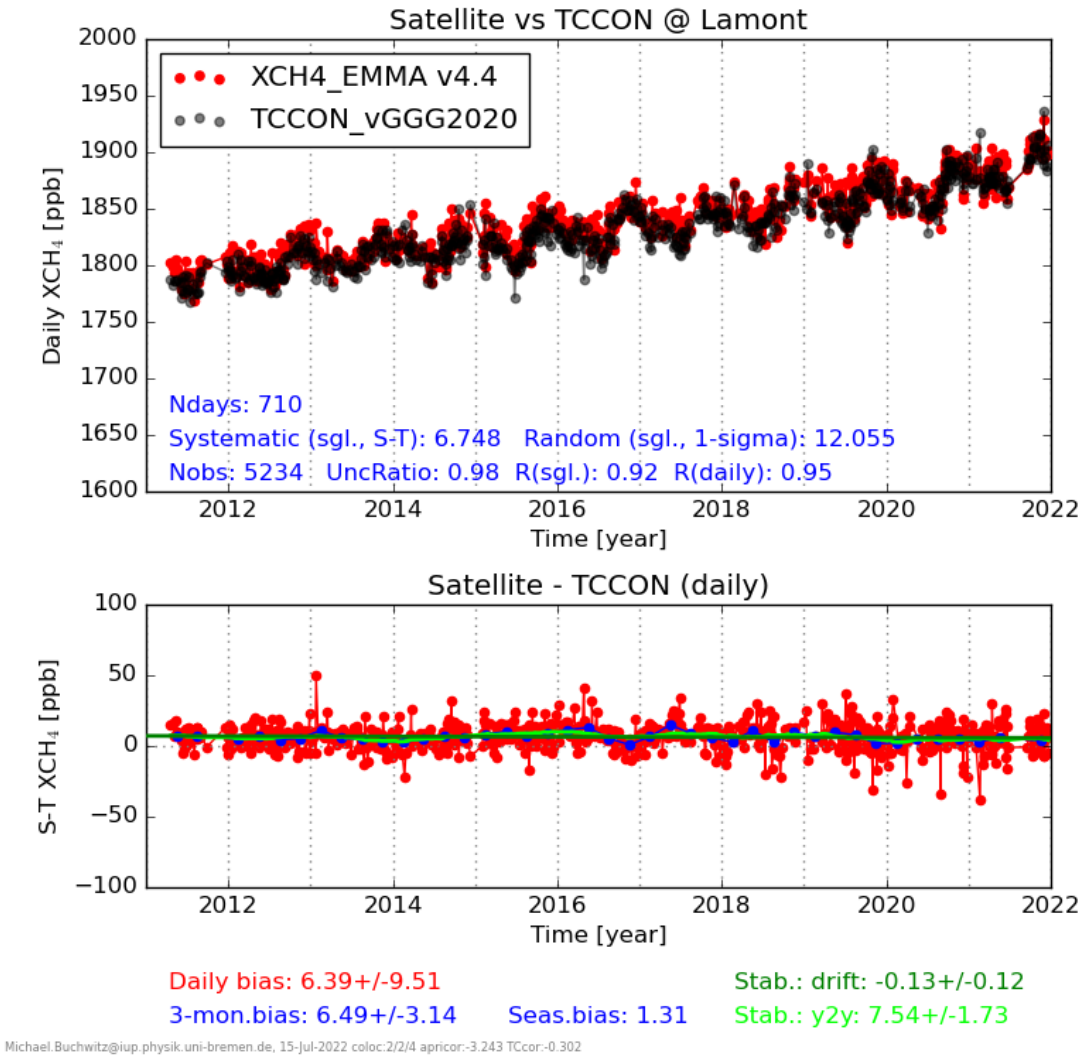
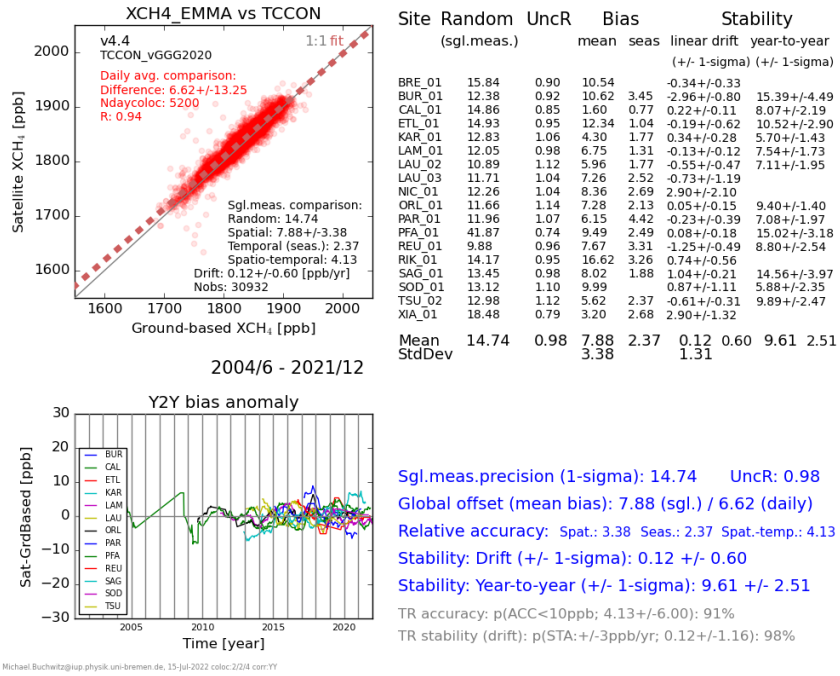


Figure 20 – As Figure 6 but for product XCH4_EMMA.



Site	Random (sgl.meas.)	UncR	Bias mean	Bias seas	Stability linear drift (+/- 1-sigma)	Stability year-to-year (+/- 1-sigma)
BRE_01	15.84	0.90	10.54		-0.34+/-0.33	
BUR_01	12.38	0.92	10.62	3.45	-2.96+/-0.80	15.39+/-4.49
CAL_01	14.86	0.85	1.60	0.77	0.22+/-0.11	8.07+/-2.19
ETL_01	14.93	0.95	12.34	1.04	-0.19+/-0.62	10.52+/-2.90
KAR_01	12.83	1.06	4.30	1.77	0.34+/-0.28	5.70+/-1.43
LAM_01	12.05	0.98	6.75	1.31	-0.13+/-0.12	7.54+/-1.73
LAU_02	10.89	1.12	5.96	1.77	-0.55+/-0.47	7.11+/-1.95
LAU_03	11.71	1.04	7.26	2.52	-0.73+/-1.19	
NIC_01	12.26	1.04	8.36	2.69	2.90+/-2.10	
ORL_01	11.66	1.14	7.28	2.13	0.05+/-0.15	9.40+/-1.40
PAR_01	11.96	1.07	6.15	4.42	-0.23+/-0.39	7.08+/-1.97
PFA_01	41.87	0.74	9.49	2.49	0.08+/-0.18	15.02+/-3.18
REU_01	9.88	0.96	7.67	3.31	-1.25+/-0.49	8.80+/-2.54
RIK_01	14.17	0.95	16.62	3.26	0.74+/-0.56	
SAG_01	13.45	0.98	8.02	1.88	1.04+/-0.21	14.56+/-3.97
SOD_01	13.12	1.10	9.99		0.87+/-1.11	5.88+/-2.35
TSU_02	12.98	1.12	5.62	2.37	-0.61+/-0.31	9.89+/-2.47
XIA_01	18.48	0.79	3.20	2.68	2.90+/-1.32	
Mean	14.74	0.98	7.88	2.37	0.12	0.60	9.61	2.51
StdDev			3.38		1.31			

Sgl.meas.precision (1-sigma): 14.74 UncR: 0.98
Global offset (mean bias): 7.88 (sgl.) / 6.62 (daily)
Relative accuracy: Spat.: 3.38 Seas.: 2.37 Spat.-temp.: 4.13
Stability: Drift (+/- 1-sigma): 0.12 +/- 0.60
Stability: Year-to-year (+/- 1-sigma): 9.61 +/- 2.51
TR accuracy: p(ACC<10ppb; 4.13+/-6.00): 91%
TR stability (drift): p(STA:+/-3ppb/yr; 0.12+/-1.16): 98%

Table 10 - Product Quality Summary Table for product XCH4_EMMA.

Product Quality Summary Table for Product: XCH4_EMMA Level: 2, Version: 4.4, Time period covered: 01.2003 – 12.2021				
Parameter [unit]	Achieved performance	Requirement	TR	Comments
Single measurement precision (1-sigma) in [ppb]	14.7	< 34 (T) < 17 (B) < 9 (G)	-	-
Uncertainty ratio) in [-]: Ratio reported uncertainty to standard deviation of satellite-TCCON difference	0.98	-	-	No requirement but value close to unity expected for a high quality data product.
Mean bias [ppb]	7.88	-	-	No requirement but value close to zero expected for a high quality data product.
Accuracy: Relative systematic error [ppb]	Spatial – spatiotemporal: 3.9 – 4.1	< 10	Probability that accuracy TR is met: 91%	-
Stability: Linear bias trend [ppb/year]	0.12 +/- 0.60 (1-sigma)	< 3	Probability that stability TR is met: 98%	-
Stability: Year-to-year bias variability [ppb/year]	9.6 +/- 2.5 (1-sigma)	< 3	-	-

2.3 Validation results for Level 3 XCO_2 product

In order to validate this product, it has been compared with the Total Carbon Column Observation Network (TCCON, Wunch et al., 2011) ground-based XCO_2 retrievals using version GGG2014 (Wunch et al., 2015) or the recently (end of April 2022) released version GGG2020 (https://tccon-wiki.caltech.edu/Main/GGG2020DataChanges) (Laughner et al., 2021).

The validation has been done in a similar way to the Level 2 products but with some exceptions, e.g., the monthly mean product has been directly compared with monthly mean TCCON data. Figure 21 shows an overview of all validation results whilst Table 11 shows the product quality summary table for this product.

The validation of Level 3 product XCO2_OBS4MIPS can be summarized as follows: The overall monthly mean uncertainty is 1.1 ppm and the mean bias is 0.28 ppm. Relative systematic errors, i.e., spatial and temporal biases amount to 0.5±0.6 ppm. The computed linear drift of 0.09±0.23 ppm is small and not significant. The probability that the 0.5 ppm accuracy requirement is met is 68%. The probability that the 0.5 ppm/year stability requirement is met is 95%. Overall, this product has therefore good accuracy and high stability.

Figure 21 – Overview validation results product XCO2_OBS4MIPS.

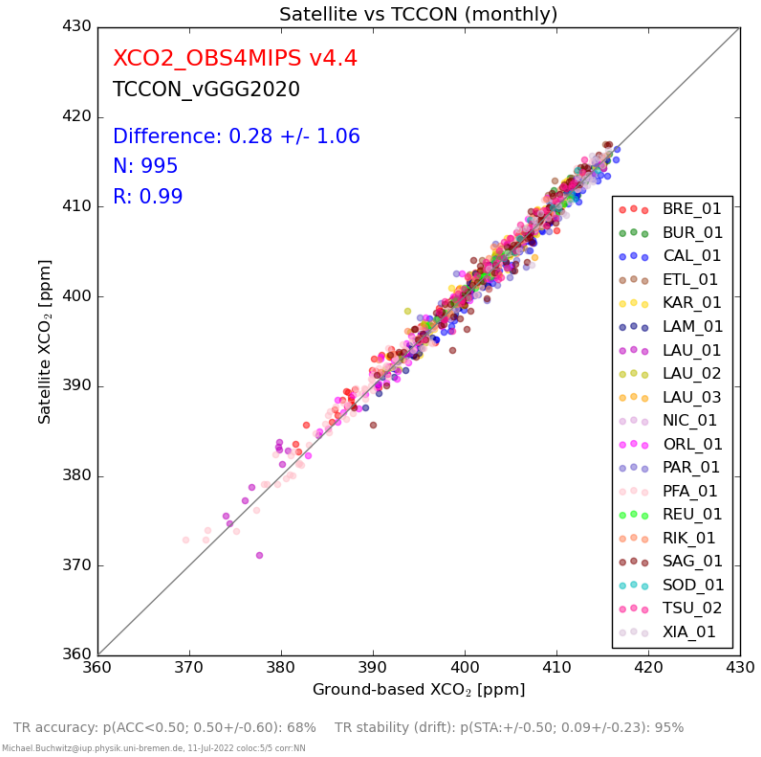


Table 11 – Product Quality Summary Table for product XCO2_OBS4MIPS.

Product Quality Summary Table for Product: XCO2_OBS4MIPS Level: 3, Version: 4.4, Time period covered: 01.2003 – 12.2021				
Parameter [unit]	Achieved performance	Requirement	TR	Comments
Overall uncertainty [ppm]	1.1	-	-	No requirement but small value expected for a high quality data product.
Mean bias [ppm]	0.28	-	-	No requirement but value close to zero expected for a high quality data product.
Accuracy: Relative systematic error [ppm]	Spatio-temporal bias: 0.5 +/- 0.6 (1-sigma)	< 0.5	Probability that accuracy TR is met: 68%	-
Stability: Linear bias trend [ppm/year]	0.09 +/- 0.23 (1-sigma)	< 0.5	Probability that stability TR is met: 95%	-

2.4 Validation results for Level 3 XCH_4 products

In order to validate this product, it has been compared with Total Carbon Column Observation Network (TCCON, Wunch et al., 2011) ground-based XC_{H4} retrievals using version GGG2014 (Wunch et al., 2015) or the recently (end of April 2022) released version GGG2020 (https://tccon-wiki.caltech.edu/Main/GGG2020DataChanges) (Laughner et al., 2021).

The validation has been done similarly as for the Level 2 products but with some exception, e.g., the monthly mean product has been directly compared with monthly mean TCCON data.

Figure 22 shows an overview of all validation results.

Table 12 shows the product quality summary table for this product.

The validation of Level 3 product XCH4_OBS4MIPS can be summarized as follows: The overall monthly mean uncertainty is 7.9 ppb and the mean bias is 4.4 ppb. Relative systematic errors, i.e., spatial and temporal biases amount to 4.7±6 ppb. The computed linear drift of 0.45±1.2 ppb is small and not significant. The probability that the 10 ppb accuracy requirement is met is 89%.
The probability that the 3 ppb/year stability requirement is met is 98%. Overall, this product has therefore very good accuracy and high stability.

Figure 22 – Overview validation results product XCH4_OBS4MIPS.

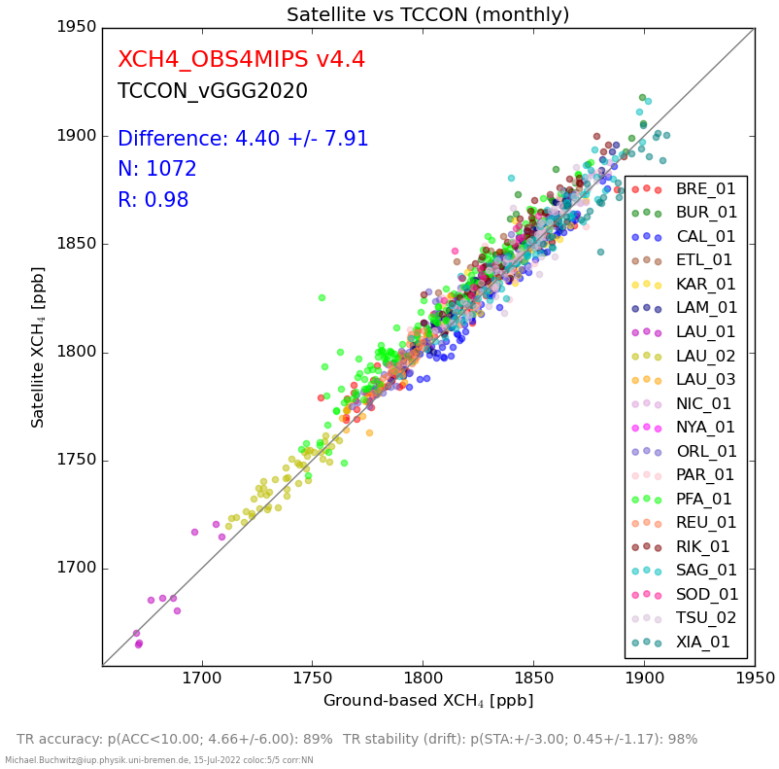


Table 12 – Product Quality Summary Table for product XCH4_OBS4MIPS.

Product Quality Summary Table for Product: XCH4_OBS4MIPS Level: 3, Version: 4.4, Time period covered: 01.2003 – 12.2021				
Parameter [unit]	Achieved performance	Requirement	TR	Comments
Overall uncertainty [ppm]	7.9	-	-	No requirement but small value expected for a high quality data product.
Mean bias [ppb]	4.4	-	-	No requirement but value close to zero expected for a high quality data product.
Accuracy: Relative systematic error [ppb]	Spatio-temporal bias: 4.7 +/- 6.0 (1-sigma)	< 10	Probability that accuracy TR is met: 89%	-
Stability: Linear bias trend [ppb/year]	0.45 +/- 1.17 (1-sigma)	< 3	Probability that stability TR is met: 99%	-

2.5 Validation results for Level 2 mid-tropospheric products

Detailed validation results are given in Annex E to this document. A summary of the validation results is given in Table 13 and Table 14.

Summary quality IASI CO_2 products:

The single measurement precision of product CO2_IASA_NLIS (from IASI on Metop-A) is 1 ppm. The mean bias (global offset) is 0.96 ppm. The estimated relative accuracy is around 1 ppm. The probability that the < 0.5 ppm user requirement is met has been estimated to 50% taking into account the uncertainty of the reference data and assessment method. The product is also very stable (0.06 +/- 0.10 ppm/year (1-sigma)) meeting the requirement for long-term drift stability. The performance of product CO2_IASB_NLIS (from IASI on Metop-B) is similar.

Summary quality IASI CH_4 products:

The single measurement precision of product CH4_IASA_NLIS (from IASI on Metop-A) is 12 ppb. The mean bias (global offset) is -3.4 ppb. The product appears to meet the “relative systematic error” requirement of better than 10 ppb: the estimated relative accuracy is 3.4 ppb. The product appears to be very stable but a quantitative analysis could not be carried out due to lack of reference data. The performance of product CH4_IASB_NLIS (from IASI on Metop-B) is similar.

Table 13 - Product Quality Summary Table for product CO2_IASA_NLIS.

Product Quality Summary Table for Product: CO2_IASA_NLIS Level: 2, Version: 9.1, Time period covered: 7.2007 – 12.2021				
Parameter [unit]	Achieved performance	Requirement	TR	Comments
Single measurement precision (1-sigma) in [ppm]	0.99	< 8 (T) < 3 (B) < 1 (G)	-	-
Mean bias [ppm]	0.96	-	-	No requirement but value close to zero expected for a high quality data product.
Accuracy: Relative systematic error [ppm]	Spatial – spatiotemporal: 0.96 / 1.09	< 0.5	Probability that accuracy TR is met: 50%	-
Stability: Drift [ppm/year]	0.06 ± 0.10 (1-sigma)	< 0.5	Probability that stability TR is met: 100%	-
Stability: Year-to-year bias variability [ppm/year]	2.78 ± 0.81 (1-sigma)	< 0.5	-	-

Table 14 - Product Quality Summary Table for products CH4_IASA_NLIS (NC stands for Not computed due to lack of available data).

Product Quality Summary Table for Product: CH4_IASA_NLIS Level: 2, Version: 9.1, Time period covered: 7.2007 – 12.2021				
Parameter [unit]	Achieved performance	Requirement	TR	Comments
Single measurement precision (1-sigma) in [ppb]	11.8	< 34 (T) < 17 (B) < 9 (G)	-	-
Mean bias [ppb]	-3.38	-	-	No requirement but value close to zero expected for a high quality data product.
Accuracy: relative systematic error [ppb]	3.38	< 10	Probability that accuracy TR is met: 90%	-
Stability: Linear bias trend [ppb/year]	NC	< 3	NC	Time series of available aircraft/AirCore obs are not long enough to compute these 2 parameters
Stability: Year-to-year bias variability [ppb/year]	NC	< 3	-	

3. Application(s) specific assessments

The new data products validated in this document and its ANNEXes have not yet been used for application specific assessments in terms of peer-reviewed publications.

However, the new XCO_2 and XCH_4 v4.4 OBS4MIPS products have already been used for a Copernicus Press Release issued on 9-January-2023: “Copernicus: 2022 was a year of climate extremes, with record high temperatures and rising concentrations of greenhouse gases” (https://climate.copernicus.eu/copernicus-2022-was-year-climate-extremes-record-high-temperatures-and-rising-concentrations) and for “Global Climate Highlights 2022” (https://climate.copernicus.eu/global-climate-highlights-2022).

4. Compliance with user requirements

The user requirements are listed in the Target Requirement and Gap Analysis Document (D4).

This section summarizes the achieved data quality including comparisons with the required data quality.

4.1 Summary data quality Level 2 XCO_2 products

Figure 27 shows a summary of the achieved performance in terms of single measurement precision, (relative) accuracy (in terms of spatial and spatio-temporal biases) and stability (in terms of linear bias drift / trend).

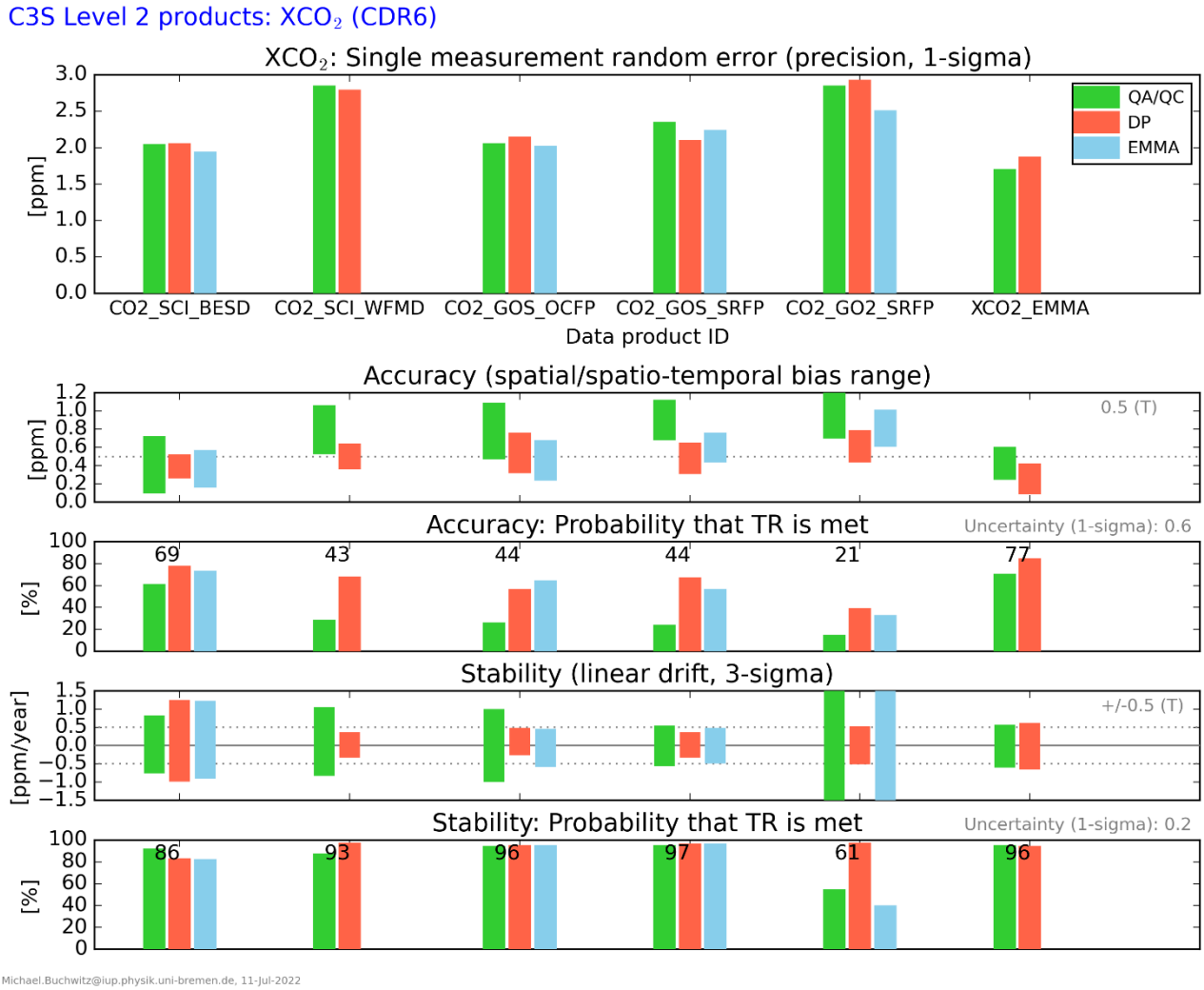
Note that this figure contains for completeness results from previous assessments for CDR5 for products not updated for CDR6. These products are: SCIAMACHY products and SRON GOSAT products. See corresponding CDR5 documents (ATBD GHG, 2021; PQAR GHG, 2021; PUGS GHG, 2021).

As can be seen, the achieved single observation random error (or precision) is typically close to 2 ppm and better than 3 ppm for all products. This is better than the required breakthrough requirement (B) of better than 3 ppm but somewhat worse than the goal (G) requirement of better than 1 ppm.

The systematic error (relative accuracy) threshold (T) requirement is “better than 0.5 ppm”. The achieved performance is around 0.7 ppm +/- a few 0.1 ppm, depending on product and assessment method. The probability that the threshold requirement is met is 44% for product CO2_GOS_OCFP, 21% for CO2_GO2_SRFP and 77% for XCO2_EMMA.

Stability is very good. No significant linear bias drift has been detected. The probability that the threshold (T) stability requirement of 0.5 ppm/year is met is close to 100% percent for all product except for product CO2_GO2_SRFP (61%).

Figure 23 - Overview data quality assessment results for Level 2 XCO_2 data products. The green bars refer to the "Quality Assessment / Quality control" (QA/QC) results as described in this document. The red bars refer to results obtained by the data providers (DPs), as described in separate Annexes (see Sect. 6). The blue bars result from an assessment using the EMMA method (see Sect. 2.1.3). For "Accuracy" and "Stability" also the numerical values for the "Probability that TR is met" are given (computed as mean value if more than one value (bar) exists). Also listed (in grey on the right hand side) is the uncertainty of the reference data as used for the Target Requirements (TR) assessment. The listed values for products generated in previous C3S projects (products CO2_SCI_BESD, CO2_SCI_WFMD and CO2_GOS_SFFP) are listed here for completeness but have not been updated (for details see *PQAR GHG, 2021*).



4.2 Summary data quality Level 2 XCH_4 products

Figure 28 shows a summary of the achieved performance in terms of single measurement precision, (relative) accuracy (in terms of spatial and spatio-temporal biases) and stability (in terms of linear bias drift / trend).

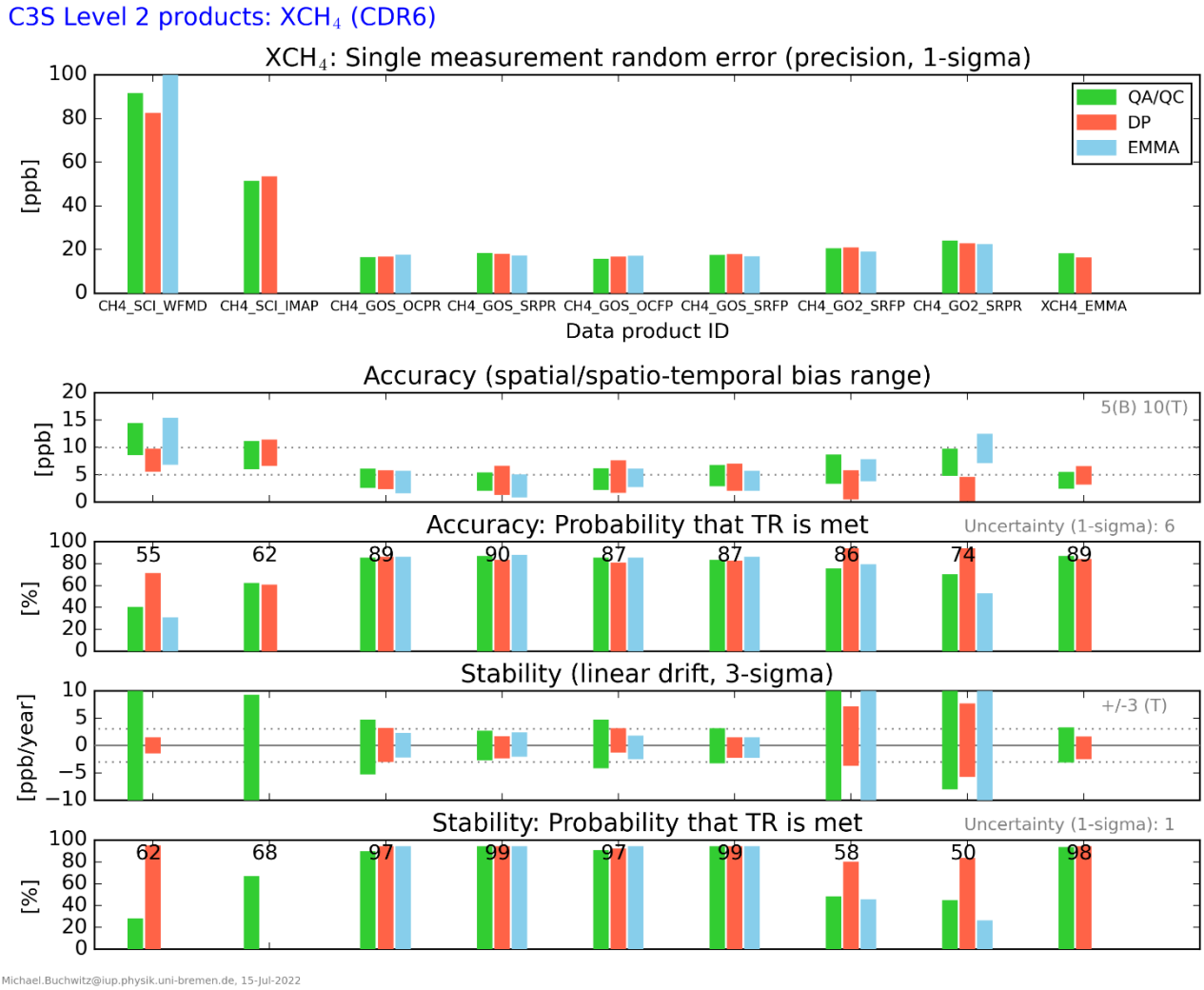
Note that this figure contains for completeness results from previous assessments for CDR5 for products not updated for CDR6. These products are: SCIAMACHY products and SRON GOSAT products. See corresponding CDR5 documents (ATBD GHG, 2021; PQAR GHG, 2021; PUGS GHG, 2021).

As can be seen, the achieved single observation random error (or precision) is close to 17 ppb, which is the breakthrough (B) requirement, for the GOSAT and the EMMA products. For product CH4_GO2_SRFP the precision is near 20 ppb and for product CH4_GO2_SRPR the precision is slightly larger than 20 ppb.

The systematic error (relative accuracy) threshold (T) requirement is “better than 10 ppb”. The achieved performance is around 5 ppb for the GOSAT and the EMMA products and product CH4_GO2_SRFP. For product CH4_GO2_SRPR the estimated accuracy depends on assessment method and is in the range 5 – 10 ppb.

Stability is very good for all GOSAT products and the EMMA product. For these products no significant linear bias drift has been detected. The probability that the threshold (T) stability requirement of 3 ppb/year is met is close to 100% for these products. The probability is much less for the two GOSAT-2 products (58% for the FP product and 50% for the PR product, but note that these products only cover relatively short time periods).

Figure 24 - Overview data quality assessment results for Level 2 XCH_2 data products. The green bars refer to the "Quality Assessment / Quality control" (QA/QC) results as described in this document. The red bars refer to results obtained by the data providers (DPs), as described in separate Annexes (see Sect. 6). The blue bars result from an assessment using the EMMA method (see Sect. 2.2.5). For "Accuracy" and "Stability" also the numerical values for the "Probability that TR is met" are given (computed as mean value if more than one value (bar) exists). Also listed (in grey on the right hand side) is the uncertainty of the reference data as used for the Target Requirements (TR) assessment. The listed values for products generated in previous C3S projects (products CH4_SCI_WFMD, CH4_SCI_IMAP, CH4_GOS_SRFP and CH4_GOS_SFPR) are listed here for completeness but have not been updated (for details see *PQAR GHG, 2021*).



4.3 Summary data quality Level 3 XCO_2 product

The validation of Level 3 product XCO2_OBS4MIPS can be summarized as follows: The overall monthly mean uncertainty is 1.1 ppm and the mean bias is 0.28 ppm. Relative systematic errors, i.e., spatial and temporal biases amount to 0.5±0.6 ppm. The computed linear drift of 0.09±0.23 ppm is small and not significant.

The probability that the 0.5 ppm accuracy requirement is met is 68%.

The probability that the 0.5 ppm/year stability requirement is met is 95%.

Overall, this product has therefore reasonable accuracy and high stability.

4.4 Summary data quality Level 3 XCH_4 product

The validation of Level 3 product XCH4_OBS4MIPS can be summarized as follows: The overall monthly mean uncertainty is 7.9 ppb and the mean bias is 4.4 ppb. Relative systematic errors, i.e., spatial and temporal biases amount to 4.7±6 ppb. The computed linear drift of 0.45±1.2 ppb is small and not significant.

The probability that the 10 ppb accuracy requirement is met is 89%.

The probability that the 3 ppb/year stability requirement is met is 98%.

Overall, this product has therefore very good accuracy and high stability.

4.5 Summary data quality Level 2 mid-tropospheric CO_2 products

The single measurement precision of product CO2_IASA_NLIS (from IASI on Metop-A) is 1 ppm. The mean bias (global offset) is 0.96 ppm. The estimated relative accuracy is around 1 ppm. The probability that the < 0.5 ppm user requirement is met has been estimated to 50% taking into account the uncertainty of the reference data and assessment method. The product is also very stable (0.06 +/- 0.10 ppm/year (1-sigma)) meeting the requirement for long-term drift stability. The performance of product CO2_IASB_NLIS (from IASI on Metop-B) is similar.

4.6 Summary data quality Level 2 mid-tropospheric CH_4 products

The single measurement precision of product CH4_IASA_NLIS (from IASI on Metop-A) is 12 ppb. The mean bias (global offset) is -3.4 ppb. The product appears to meet the “relative systematic error” requirement of better than 10 ppb: the estimated relative accuracy is 3.4 ppb. The product appears to be very stable but a quantitative analysis could not be carried out due to lack of reference data. The performance of product CH4_IASB_NLIS (from IASI on Metop-B) is similar.

4.7 Overall summary data quality all products

Table 17 provides and overview of all products and their estimated data quality in terms of Target Requirement (TR) assessments.

Table 15 - Overview quality assessment results of products in terms of Target Requirements (TRs). For additional quality assessment results see Figure 27 and Figure 28.

Product ID	Level	Description	Probability that TR is met		Details see Sect.
			Accuracy	Stability	
XCO_2 products			Required: < 0.5 ppm	Required: < 0.5 ppm/year	
CO2_GOS_OCFP	2	XCO_2 from GOSAT retrieved using Univ. Leicester's OCFP algorithm	44%	96%	3.1.1
CO2_GO2_SRFP	2	XCO_2 from GOSAT-2 retrieved using SRON's SRFP (RemoTeC) algorithm	21%	61%	3.1.2
XCO2_EMMA	2	Merged multi-satellite XCO_2 via Univ. Bremen's EMMA algorithm	77%	96%	3.1.3
XCO2_OBS4MIPS	3	Merged multi-satellite XCO_2 via Univ. Bremen's OBS4MIPS algorithm	68%	95%	3.3

Product ID	Level	Description	Probability that TR is met		Details see Sect.
			Accuracy	Stability	
XCH_4 products			Required: < 10 ppb	Required: < 3 ppb/year	
CH4_GOS_OCFP	2	XCH_4 from GOSAT retrieved using Univ. Leicester's OCFP algorithm	87%	97%	3.2.1
CH4_GOS_OCPR	2	XCH_4 from GOSAT retrieved using Univ. Leicester's OCPR algorithm	89%	97%	3.2.2
CH4_GO2_SRFP	2	XCH_4 from GOSAT-2 retrieved using SRON's SRFP (RemoTeC) algorithm	86%	58%	3.2.3
CH4_GO2_SRPR	2	XCH_4 from GOSAT-2 retrieved using SRON's SRPR (RemoTeC) algorithm	74%	50%	3.2.4
XCH4_EMMA	2	Merged multi-satellite XCH_4 via Univ. Bremen's EMMA algorithm	89%	98%	3.2.5
XCH4_OBS4MIPS	3	Merged multi-satellite XCH_4 via Univ. Bremen's OBS4MIPS algorithm	89%	98%	3.4

Table continued on next page …

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Product ID	Level	Description	Probability that TR is met		Details see Sect.
			Accuracy	Stability	
Mid/upper troposphere CO_2 products			Required: < 0.5 ppm	Required: < 0.5 ppm/year	
COS_IASA_NLIS	2	LMD's product from IASI/Metop-A	50%	100%	3.5
CO2_IASB_NLIS	2	LMD's product from IASI/Metop-B	-	-	3.5
Mid/upper troposphere CH_4 products			Required: < 10 ppb	Required: < 3 ppb/year	
CH4_IASA_NLIS	2	LMD's product from IASI/Metop-A	90%	-	3.5
CH4_IASB_NLIS	2	LMD's product from IASI/Metop-B	-	-	3.5

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We also acknowledge the availability of OCO-2 Level 1 and Level 2 (XCO_2) data products from NASA, which have been used for the generation on the XCO2_EMMA and XCO2_OBS4MIPS products. These products also include OCO-2 XCO_2 retrieved at Univ. Bremen with the FOCAL algorithm. The FOCAL activities would not have been possible without funding from University of Bremen, from the EU H2020 projects CHE (grant agreement ID: 776186) and VERIFY (Grant agreement ID: 776810), from ESA via project GHG-CCI+ and from EUMETSAT project FOCAL-CO2M.

Last but not least we acknowledge the availability of TCCON data via the TCCON data archive (https://tccondata.org/).

6. List of ANNEXes

The ANNEXes to this main document are the following ANNEXes A – E:

6.1 ANNEX A: PQAR for products CO2_GOS_OCFP, CH4_GOS_OCFP, CH4_OCPR

Describes the validation of the GOSAT XCO_2 and XCH_4 Level 2 products generated by University of Leicester, UK.

6.2 ANNEX B: PQAR for products CO2_GO2_SRFP, CH4_GO2_SRFP

Describes the validation of the GOSAT-2 XCO_2 and XCH_4 Full Physics (FP) Level 2 products generated by SRON, The Netherlands.

6.3 ANNEX C: PQAR for product CH4_GO2_SRPR

Describes the validation of the GOSAT-2 XCH_4 Proxy (PR) Level 2 product generated by SRON, The Netherlands.

6.4 ANNEX D: PQAR for XCO2_EMMA, XCH4_EMMA, XCO2_OBS4MIPS, XCH4_OBS4MIPS

Describes the validation of the multi-sensor multi-algorithms merged XCO_2 and XCH_4 Level 2 and 3 products generated by University of Bremen, Germany.

6.5 ANNEX E: PQAR for IASI CO_2 and CH_4 products

Describes the validation of the mid-tropospheric CO_2 and CH_4 products from the IASI instrument series generated by LMD/CNRS, France.

These ANNEXes and the corresponding data products are / will be available via the Copernicus Climate Data Store (CDS):
https://cds.climate.copernicus.eu/#!/home

See also Copernicus Climate Change Service (C3S):
https://climate.copernicus.eu/

pdf versions of all documents (including previous versions) are (also) available from
https://www.iup.uni-bremen.de/carbon_ghg/cg_data.html#C3S_GHG

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