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Copernicus Climate Change Service

Product Quality Assessment Report (PQAR) – Main document for Greenhouse Gas (GHG: CO_2 & CH_4) data set CDR 4 (2003-2019)

C3S_312b_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
3.1	03-November-2019	Update after review by Assimila: Correction of typos and broken links. Other changes: Figures 35 and 36 updated and reference to Reuter et al., 2019, added. Updates of figures and tables in Sects. 3.1 and 3.2 to correct for a bug in the computation of "Uncertainty ratio".	First 7 pages (date, version number, etc.), update of Figs. 35 and 36, updates of figures and tables in Sects. 3.1 and 3.2.
4.0 beta	18-August-2020	Update for data set CDR4 (temporal coverage: 2003-2019)	All
4.0	17-September-2020	Several improvements after review by Assimila	All

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, 2016.
D4	**TRD GAD GHG, 2020:** Buchwitz, M., Aben, I., Armante, R., Boesch, H., Crevoisier, C., Hasekamp, O. P., Wu, L.., Reuter, M., Schneising-Weigel, O., 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 (project C3S_312b_Lot2), Version 2.11, 9-April-2020, pp. 80, 2020.
D5	**ATBD GHG, 2020:** Buchwitz, M., Aben, I., Boesch, H., Crevoisier, C., Hasekamp, O. P., Reuter, M., Schneising-Weigel, O., Wu, L.., Algorithm Theoretical Basis Document (ATBD) – Main document for Greenhouse Gas (GHG: CO_2 & CH_4) data set CDR 4 (2003-2019), C3S project C3S_312b_Lot2_DLR, v4.0, 2020.
D6	**PUGS GHG, 2020:** Buchwitz, M., Aben, I., J., Armante, R., Boesch, H., Crevoisier, C., Di Noia, A., Hasekamp, O. P., Reuter, M., Schneising-Weigel, O., Wu, L.., Product User Guide and Specification (PUGS) – Main document for Greenhouse Gas (GHG: CO_2 & CH_4) data set CDR 4 (2003-2019), C3S project C3S_312b_Lot2_DLR, v4.0, 2020.

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
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

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

Table 1 lists some general definitions relevant for this document. Other definitions, which require more detailed explanations, are given below.

Table 1 - General definitions.

Item	Definition
XCO_2	Column-average dry-air mixing ratio (mole fraction) of CO_2
XCH_4	Column-average dry-air mixing ratio (mole fraction) of CH_4
L1	Level 1 satellite data product: geolocated radiance (spectra)
L2	Level 2 satellite-derived data product: Here: CO_2 and CH_4 information for each ground-pixel
L3	Level 3 satellite-derived data product: Here: Gridded CO_2 and CH_4 information, e.g., 5 deg times 5 deg, monthly
L4	Level 4 satellite-derived data product: Here: Surface fluxes (emission and/or uptake) of CO_2 and CH_4

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 is the temporal frequency at which the measurements are required (*CMUG-RBD, 2010*).

Note: In this document also the term “Revisit time” may be used. The definition is identical with the definition of “Observing cycle”. Both terms refer to the (average) temporal frequency at a given location.

Scope of document

This document is the Product Quality Assurance 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 C3S_312b_Lot2 led by DLR, Germany (a follow-on activity of project C3S_312a_Lot6 led by University of Bremen, Germany), in the following referred to as C3S/GHG 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-average 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 2 for the CO_2 products and in Table 3 for the CH_4 products.

For an overview of the merged Level 2 data products XCO2_EMMA and XCH4_EMMA and of the merged Level 3 data products XCO2_OBS4MIPS and XCH4_OBS4MIPS see also *Reuter et al., 2019*.

Requirements on data quality are formulated in the corresponding Target Requirement Document (TRD) (*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.

Table 2: 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_SCI_BESD (L2)	02.01.02	1-4	01.2003 – 03.2012	XCO_2 from SCIAMACHY as retrieved with Univ. Bremen's BESD algorithm. Brokered from GHG-CCI.
CO2_SCI_WFMD (L2)	4.0	1-4	10.2002 – 04.2012	XCO_2 from SCIAMACHY as retrieved with Univ. Bremen's WFMD algorithm. Brokered from GHG-CCI.
CO2_GOS_OCFP (L2)	7.1 7.2 7.3	1 2-3 4	04.2009 – 12.2016 04.2009 – 12.2018 04.2009 – 12.2019	XCO_2 from GOSAT as retrieved with Univ. Leicester's OCFP algorithm.
CO2_GOS_SRFP (L2)	2.3.8	1-4	04.2009 – 12.2019	XCO_2 from GOSAT as retrieved with SRON's SRFP (RemoTeC) algorithm.
XCO2_EMMA (L2)	3.0 3.1 4.1 4.2	1 2 3 4	01.2003 – 12.2016 01.2003 – 12.2017 01.2003 – 12.2018 01.2003 – 12.2019	Merged L2 XCO_2 product using Univ. Bremen's EMMA algorithm.
XCO2_OBS4MIPS (L3)	3 3.1 4.1 4.2	1 2 3 4	01.2003 – 12.2016 01.2003 – 12.2017 01.2003 – 12.2018 01.2003 – 12.2019	Merged L3 XCO_2 product in OBS4MIPS format.
CO2_AIRS_NLIS (L2)	3.0	1-4	04.2003 – 07.2007	Mid-tropospheric CO_2 mixing ratios as retrieved from AIRS using LMD's NLIS algorithm. Brokered from GHG-CCI.
CO2_IASA_NLIS (L2)	8.0 9.1	1-3 4	7.2007 – 05.2015 7.2007 – 12.2019	Mid-tropospheric CO_2 mixing ratios as retrieved from IASI/Metop-A using LMD's NLIS algorithm.
CO2_IASB_NLIS (L2)	4.0 4.2 9.1	1 2-3 4	2.2013 – 12.2016 2.2013 – 12.2018 2.2013 – 12.2019	Mid-tropospheric CO_2 mixing ratios as retrieved from IASI/Metop-B using LMD's NLIS algorithm.

Table 3: 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_SCI_WFMD (L2)	4.0	1-4	10.2002 – 12.2011	XCH_4 from SCIAMACHY as retrieved with Univ. Bremen's WFMD algorithm. Brokered from GHG-CCI.
CH4_SCI_IMAP (L2)	7.2	1-4	01.2003 – 04.2012	XCH_4 from SCIAMACHY as retrieved with SRON/JPL's IMAP algorithm. Brokered from GHG-CCI.
CH4_GOS_OCPR (L2)	7.0 7.2 7.3	1 2-3 4	04.2009 – 12.2016 04.2009 – 12.2018 04.2009 – 12.2019	XCH_4 from GOSAT as retrieved with Univ. Leicester's OCPR algorithm.
CH4_GOS_SRPR (L2)	2.3.8 2.3.9	1 2-4	04.2009 – 12.2016 04.2009 – 12.2019	XCH_4 from GOSAT as retrieved with SRON's SRPR (RemoTeC) algorithm.
CH4_GOS_OCFP (L2)	7.1 7.2 7.3	1 2-3 4	04.2009 – 12.2016 04.2009 – 12.2018 04.2009 – 12.2019	XCH_4 from GOSAT as retrieved with Univ. Leicester's OCFP algorithm.
CH4_GOS_SRFP (L2)	2.3.8 2.3.8	1 2-4	04.2009 – 12.2016 04.2009 – 12.2019	XCH_4 from GOSAT as retrieved with SRON's SRFP (RemoTeC) algorithm.
XCH4_EMMA (L2)	3.0 3.1 4.1 4.2	1 2 3 4	01.2003 – 12.2016 01.2003 – 12.2017 01.2003 – 12.2018 01.2003 – 12.2019	Merged L2 XCH_4 product using Univ. Bremen's EMMA algorithm.
XCH4_OBS4MIPS (L3)	3 3.1 4.1 4.2	1 2 3 4	01.2003 – 12.2016 01.2003 – 12.2017 01.2003 – 12.2018 01.2003 – 12.2019	Merged L3 XCH_4 product in OBS4MIPS format.
CH4_IASA_NLIS (L2)	8.4 9.1	1-3 4	7.2007 – 05.2015 7.2007 – 05.2019	Mid-tropospheric CH_4 mixing ratios as retrieved from IASI/Metop-A using LMD's NLIS algorithm.
CH4_IASB_NLIS (L2)	8.1 8.1 9.1	1 2-3 4	2.2013 – 12.2016 2.2013 – 12.2018 2.2013 – 12.2019	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 C3S_312b_Lot2 project of the Copernicus Climate Change Service (C3S, https://climate.copernicus.eu/) is described.

The C3S_312b_Lot2 satellite-derived greenhouse gas (GHG) data products are:

- Column-average 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).

These data products are generated from the satellite instruments SCIAMACHY/ENVISAT and TANSO-FTS/GOSAT (XCO_2 and XCH_4 products) and AIRS and IASI (mid/upper troposphere products). For the products XCO2_EMMA and XCO2_OBS4MIPS also Level 2 products from NASA's OCO-2 mission have been used as input products (see also *Reuter et al., 2020*). All data products are available as Level 2 (individual ground pixels) products in NetCDF format. 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 (currently about 400 ppm for CO_2 and 1.8 ppm (1800 ppb) for CH_4) 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 Document (*TRD, 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 C3S_312a_Lot6 project is essentially the (pre-)operational continuation of the research and development (R&D) pre-cursor project GHG-CCI of ESA's Climate Change Initiative (CCI). The main goal of the C3S_312b_Lot2 project (and its C3S_312a_Lot6 pre-cursor project) is to extend (in time) the data base of ESA GHG-CCI pre-cursor data products.

The first C3S_312a_Lot6 GHG data set - Climate Data Record 1 (CDR1) - covered the time period 2003-2016 and had been delivered to ECMWF in 2017. CDR2 covers the time period 2003-2017. The latest data set - Climate Data Record 4 (CDR4) - covers the time period 2003-2019. This document is an update for data set CDR4.

This document is the MAIN PQAR document. It provides an overview of all products including validation / quality assessment results (including the latest versions of SCIAMACHY XCO_2 and XCH_4 products as generated in the framework of the GHG-CCI project). Additional detailed validation results for each product are provided in separate ANNEXes:

- 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_GOS_SRFP, CH4_GOS_SRFP (SRON's "full physics" GOSAT products)
- ANNEX C: PQAR for product CH4_GOS_SRPR (SRON's "proxy" GOSAT 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)

Table 4 provides and overview about all products and their estimated data quality in terms of Target Requirement (TR) assessments.

Figure 1 presents an overview of the achieved data quality for all Level 2 XCO_2 data products and Figure 2 presents this overview for the Level 2 XCH_4 data products.

The validation of Level 3 product XCO2_OBS4MIPS can be summarized as follows: The overall monthly mean uncertainty is 1.2 ppm and the mean bias is -0.11 ppm. Relative systematic errors, i.e., spatial and temporal biases amount to 0.7±0.6 ppm. The computed linear drift of -0.07±0.20 ppm is small and not significant.

The validation of Level 3 product XCH4_OBS4MIPS can be summarized as follows: The overall monthly mean uncertainty is 8.8 ppb and the mean bias is -3.3 ppb. Relative systematic errors, i.e., spatial and temporal biases amount to 5±6 ppb. The computed linear drift of 0.1±1.0 ppb is small and not significant.

Table 4 - Overview quality assessment results of products in terms of Target Requirements (TRs). For additional quality assessment results see the following two figures.

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_SCI_BESD	2	XCO_2 from SCIAMACHY retrieved using Univ. Bremen's BESD algorithm	69%	86%	3.1.1
CO2_SCI_WFMD	2	XCO_2 from SCIAMACHY retrieved using Univ. Bremen's WFMD algorithm	43%	93%	3.1.2
CO2_GOS_OCFP	2	XCO_2 from GOSAT retrieved using Univ. Leicester's OCFP algorithm	46%	97%	3.1.3
CO2_GOS_SRFP	2	XCO_2 from GOSAT retrieved using SRON's SRFP (RemoTeC) algorithm	44%	97%	3.1.4
XCO2_EMMA	2	Merged multi-satellite XCO_2 via Univ. Bremen's EMMA algorithm	65%	98%	3.1.7
XCO2_OBS4MIPS	3	Merged multi-satellite XCO_2 via Univ. Bremen's OBS4MIPS algorithm	49%	97%	3.3
XCH_4 products			Required: < 10 ppb	Required: < 3 ppb/year	
CH4_SCI_WFMD	2	XCH_4 from SCIAMACHY retrieved using Univ. Bremen's WFMD algorithm	55%	62%	3.2.1
CH4_SCI_IMAP	2	XCH_4 from SCIAMACHY retrieved using the IMAP algorithm of SRON/JPL	62%	68%	3.2.2

CH4_GOS_OCPR	2	XCH_4 from GOSAT retrieved using Univ. Leicester's OCPR algorithm	89%	99%	3.2.3
CH4_GOS_SRPR	2	XCH_4 from GOSAT retrieved using SRON's SRPR (RemoTeC) algorithm	92%	99%	3.2.4
CH4_GOS_OCFP	2	XCH_4 from GOSAT retrieved using Univ. Leicester's OCFP algorithm	88%	97%	3.2.5
CH4_GOS_SRFP	2	XCH_4 from GOSAT retrieved using SRON's SRFP (RemoTeC) algorithm	87%	90%	3.2.6
XCH4_EMMA	2	Merged multi-satellite XCH_4 via Univ. Bremen's EMMA algorithm	90%	99%	3.2.7
XCH4_OBS4MIPS	3	Merged multi-satellite XCH_4 via Univ. Bremen's OBS4MIPS algorithm	88%	99%	3.4
Mid/upper troposphere CO_2 products			Required: < 0.5 ppm	Required: < 0.5 ppm/year	
CO2_AIR_NLIS	2	LMD's product from AIRS	-	-	3.5
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

Figure 1 - 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. 7). The blue bars result from an assessment using the EMMA method (see Sect. 3.1.5). 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) assessments. The DP values for the "GHG-CCI brokered products" CO2_SCI_BESD and CO2_SCI_WFM are from *Buchwitz et al., 2017*.

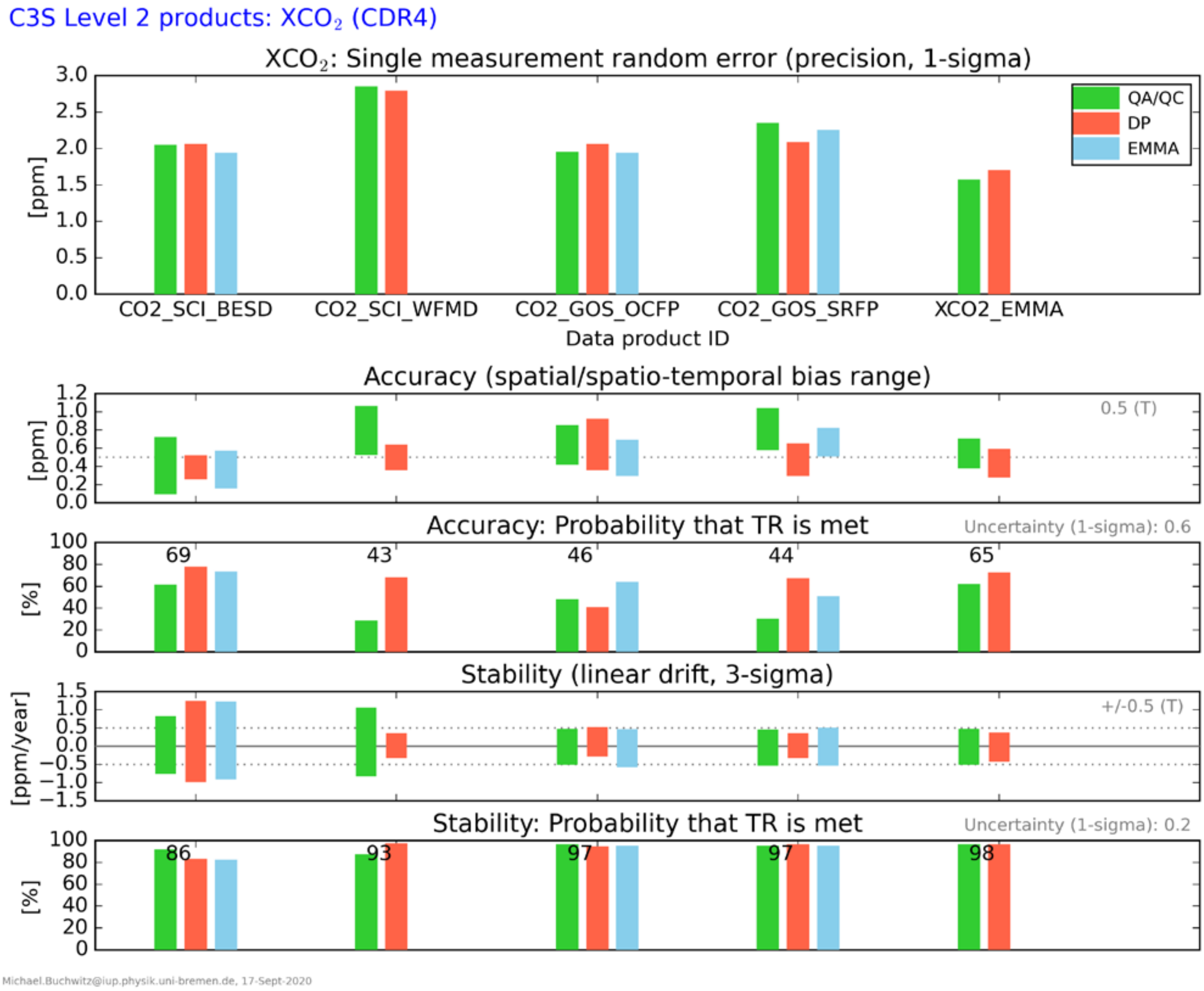


Figure 2 - Overview data quality assessment results for Level 2 XCH_2 data products. The green bars refer to the “Quality Assessment / Quality control” (QA/QC) results as described in this document. The red bars refer to results obtained by the data providers (DPs), as described in separate Annexes (see Sect. 7). The blue bars result from an assessment using the EMMA method (see Sect. 3.2.7). 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) assessments. The DP values for the “GHG-CCI brokered products” CH4_SCI_WFMD and CH4_SCI_IMAP are from *Buchwitz et al., 2017*.

1. Overview data products and instruments

In this section an overview of the data products - specified in terms of variable, its property, processing level(s) and instrument(s) - is given.

The data products are (see also *Buchwitz et al., 2013b, 2016, 2017; Reuter et al., 2020*):

- Column-average 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).
- Mid/upper tropospheric mixing ratios of CO_2 and CH_4.

Carbon dioxide and methane are important atmospheric greenhouse gases (e.g., *IPCC 2013*) but despite their importance our knowledge on their various and variable natural and anthropogenic sources and sinks has significant gaps (e.g., *IPCC 2013; Ciais et al., 2014; 2015; Kirschke et al., 2013; Nisbet et al., 2014*, and references given therein). A purpose of the satellite data products described in this document is to contribute to enhancing our knowledge on the CO_2 and CH_4 sources and sinks (via appropriate (inverse) modelling).

Carbon dioxide and methane are so-called Essential Climate Variables (ECVs) and the need to monitor them has been clearly identified along with the definition of key observational requirements (e.g., *GCOS-154, GCOS-200*). In recent years several satellite-derived ECV data products have been generated in particular in the framework of the Climate Change Initiative (CCI) of ESA (e.g., *Hollmann et al., 2013*) including CO_2 and CH_4 (e.g., *Buchwitz et al., 2013a, 2016, 2017*).

Previous version of these satellite-derived CO_2 and CH_4 data products have been used for a number of (primarily scientific) applications, e.g.,

- to improve our knowledge on the various natural and anthropogenic (surface) sources and sinks of these important greenhouse gases (GHG) (see, e.g., *Alexe et al., 2015; Bergamaschi et al., 2015; Chevallier et al., 2014, 2016a, 2016b; Cressot et al, 2014; Detmers et al., 2015; Guerlet et al., 2013; Houweling et al., 2015; McNorton et al., 2016; Pandey et al., 2016; Reuter et al., 2014b, 2017; Schneising et al., 2014b; Turner et al., 2015, 2016,* and references given therein)
- to monitor the global distribution of CO_2 and CH_4 (e.g., *Buchwitz et al., 2007, 2016b; Schneising et al., 2011; Frankenberg et al., 2011; Massart et al., 2016*)
- to improve our knowledge on emission ratios, e.g., for biomass burning (e.g., *Ross et al., 2013; Parker et al., 2016*)
- for comparisons with (chemistry) climate models (e.g., *Shindell et al., 2013; Hayman et al., 2014; Lauer et al., 2017*) and other models (e.g., *Schneising et al., 2014a; Parker et al., 2016*)

In the following sub-sections an overview about the satellite-derived CO_2 and CH_4 data products is given.

1.1 Column-average mixing ratios of CO_2 and CH_4 (XCO_2 and XCH_4)

1.1.1 Overview

Satellite radiance observations in the Near Infrared / Short Wave Infrared (NIR/SWIR) spectral region in nadir (downlooking) observation viewing mode are sensitive to atmospheric CO_2 and CH_4 concentration changes with good sensitivity down to the Earth's surface (because solar radiation reflected at the Earth's surface is observed). These measurements permit to obtain "total column information" but do not permit to obtain (detailed) information on the vertical profiles of CO_2 and CH_4. The CO_2 and CH_4 products derived from these satellites are column-averaged dry-air mixing ratios (more precisely: mole fractions) of CO_2 and CH_4 denoted XCO_2 (e.g., in ppm) and XCH_4 (e.g., in ppb).

In the following, several satellite instruments are shortly described which have been used (or will be used in the future) to generate XCO_2 and/or XCH_4 data products.

1.1.2 Instruments

In this section a short overview about relevant satellite instruments is given. The C3S data set has been primarily derived from the satellite instruments SCIAMACHY on ENVISAT and TANSO-FTS onboard GOSAT. In addition, XCO_2 from NASA's OCO-2 mission has been used for some products (EMMA and OBS4MIPS). These instruments are shortly described in the following. Other satellites are also shortly mentioned, which are planned to be used for future versions of our data products.

1.1.2.1 SCIAMACHY/ENVISAT

SCIAMACHY (SCanning Imaging Absorption spectroMeter for Atmospheric ChartographY) was a spectrometer on ESA's ENVISAT satellite (2002-2012). SCIAMACHY (*Burrows et al., 2005; Bovensmann et al., 1999*) covers the spectral region from the ultra-violet to the SWIR spectral region (240 nm - 2380 nm) at moderate spectral resolution (0.2 nm - 1.5 nm) and observes the Earth's atmosphere in various viewing geometries (nadir, limb and solar and lunar occultation). For a good general overview on SCIAMACHY see also https://en.wikipedia.org/wiki/SCIAMACHY. SCIAMACHY permits the retrieval of XCO_2 (e.g., *Reuter et al., 2011; Schneising et al., 2011*) and XCH_4 (e.g., *Schneising et al., 2011; Frankenberg et al., 2011*) from the appropriate spectral regions in the SWIR (around 1.6 µm) and the NIR (O_2 A-band at 760 nm used to obtain the dry-air column using the know dry-air mixing ratio of atmospheric oxygen). The ground pixel size is typically 30 km along track times 60 km across track and the swath width is about 960 km. There are no across-track gaps between the ground pixels but there are gaps along-track as SCIAMACHY operates only part of the time (approx. 50%) in nadir observation mode.

1.1.2.2 TANSO-FTS/GOSAT

TANSO-FTS is a Fourier-Transform-Spectrometer (FTS) onboard the Japanese GOSAT satellite (*Kuze et al., 2009, 2014, 2016*). The Greenhouse Gases Observing Satellite "IBUKI" (GOSAT) is the world's first spacecraft in orbit dedicated to measure the concentrations of carbon dioxide and methane from space. The spacecraft was launched successfully on January 23, 2009, and has been operating properly since then. GOSAT covers the relevant CO_2, CH_4 and O_2 absorption bands in the NIR and SWIR spectral region as needed for accurate XCO_2 and XCH_4 retrieval (in addition GOSAT also covers a large part of the Thermal Infrared (TIR) spectral region). The spectral resolution of TANSO-FTS is much higher compared to SCIAMACHY and also the ground pixels are smaller (10 km compared to several 10 km for SCIAMACHY). However, in contrast to SCIAMACHY, the GOSAT scan pattern consists of non-consecutive individual ground pixels, i.e., the scan pattern is not gap-free. For a good general overview about GOSAT see also http://www.gosat.nies.go.jp/en/.

GOSAT-2 has been successfully launched on 29 October 2018. OSAT-2 XCO_2 and XCH_4 retrievals are not yet included in the C3S GHG CDR.

1.1.2.3 OCO-2

NASA's Orbiting Carbon Observatory 2 (OCO-2) mission (*Crisp et al., 2004; Boesch et al., 2011*) has been successfully launched in July 2014. The OCO-2 Project primary science objective is to collect the first space-based measurements of atmospheric carbon dioxide with the precision, resolution and coverage needed to characterize its sources and sinks and quantify their variability over the seasonal cycle. During its two-year mission, OCO-2 will fly in a sun-synchronous, near-polar orbit with a group of Earth-orbiting satellites with synergistic science objectives whose ascending node crosses the equator near 13:30 hours Mean Local Time (MLT). Near-global coverage of the sunlit portion of Earth is provided in this orbit over a 16-day (233-revolution) repeat cycle. OCO-2's single instrument incorporates three high-resolution grating spectrometers, designed to measure the near-infrared absorption of reflected sunlight by carbon dioxide and molecular oxygen. OCO-2 covers similar spectral bands as SCIAMACHY and GOSAT but OCO-2 has much smaller ground pixels (km scale) but the swath width is much smaller (approx. 10 km) compared to SCIAMACHY. OCO-2 delivers XCO_2 but not XCH_4. Details on OCO-2 are also given on https://oco.jpl.nasa.gov/.

1.1.2.4 TanSat

The Chinese TanSat satellite (https://en.wikipedia.org/wiki/TanSat) has been successfully launched in December 2016. The TanSat satellite and instrument is very similar as OCO-2. As OCO-2, TanSat delivers XCO_2 but not XCH_4. TanSat XCO_2 retrievals are not yet included in the C3S GHG CDR.

1.1.2.5 Sentinel-5-Precursor (S5P)

ESA's Sentinel-5-Precursor (S5P) mission (*Veefkind et al, 2012*) has been launched in October 2017. S5P permits XCH_4 retrievals (*Butz et al., 2012, Hu et al., 2018*) at about 7 km and using a wide swath of about 2600 km. Details on S5P can also be found on https://earth.esa.int/web/guest/missions/esa-future-missions/sentinel-5P. S5P XCH_4 retrievals are not yet included in the C3S GHG CDR.

1.1.2.6 Other instruments

Several other satellites are expected to be launched in the future, e.g., the active laser-based mission MERLIN (Methane Remote Sensing Lidar Mission, see https://de.wikipedia.org/wiki/Merlin_(Satellit)).

1.1.3 XCO_2

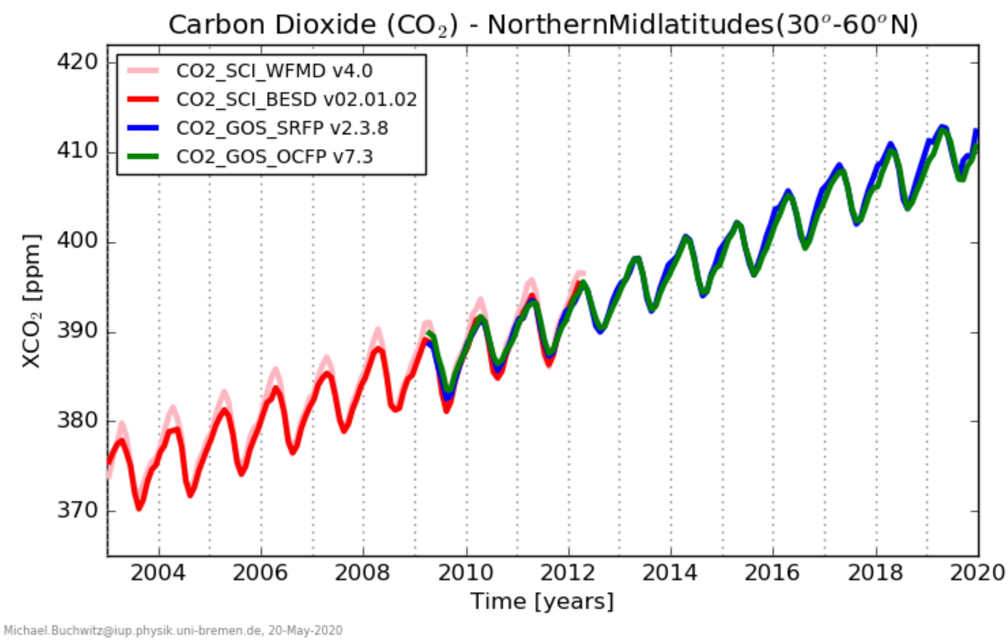
As explained, XCO_2 is the column-averaged dry-air mixing ratio (mole fraction) of atmospheric CO_2. A XCO_2 value of, for example, 400 ppm at a given location means that 400 CO_2 molecules are present in the atmosphere above that location per one million air molecules excluding water molecules.

XCO_2 can be retrieved from instruments such as SCIAMACHY/ENVISAT and TANSO-FTS/GOSAT using Optimal Estimation (*Rodgers, 2000*) or DOAS (*Buchwitz et al., 2000*) retrieval algorithms as shown in various publications (e.g., *Buchwitz et al., 2005; Butz et al., 2011; Cogan et al., 2011; Reuter et al., 2011; 2013; Schneising et al., 2011; Yoshida et al., 2013*). These products have been validated using Total Carbon Column Observing Network (TCCON) (*Wunch et al., 2010, 2011, 2015*) XCO_2 ground based observations (e.g., *Dils et al., 2014*).

In this document we describe the latest versions of these data products.

As an example, Figure 3 shows time series of satellite-derived XCO_2. As can be seen, XCO_2 is increasing by about 2 ppm/year primarily due to burning of fossil fuels and shows a pronounced seasonal cycle, primarily due to uptake and release of CO_2 by the terrestrial biosphere.

Figure 3 – Satellite-derived northern mid-latitude XCO_2 time series. Shown are four time series, each corresponding to one of the four individual satellite sensor Level 2 XCO_2 products, which are described in this document.



1.1.4 XCH_4

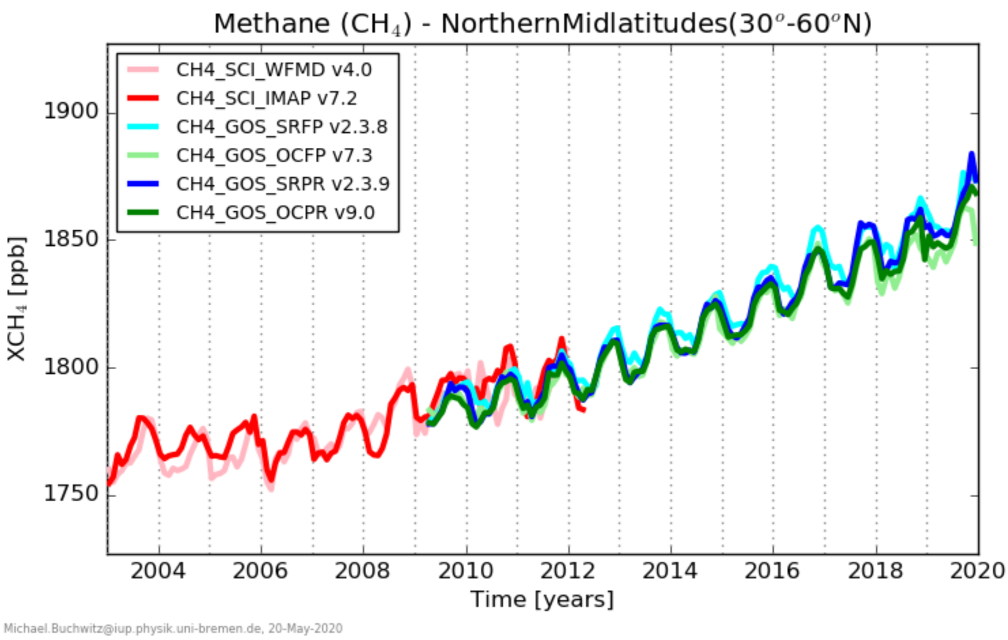
As explained, XCH_4 is the column-averaged dry-air mixing ratio (mole fraction) of atmospheric CH_4. A XCH_4 value of, for example, 1800 ppb at a given location means that 1800 CH_4 molecules are present in the atmosphere above that location per one billion air molecules excluding water molecules.

XCH_4 can be retrieved from instruments such as SCIAMACHY/ENVISAT and TANSO-FTS/GOSAT using Optimal Estimation (*Rodgers, 2000*) or DOAS (*Buchwitz et al., 2000*) retrieval algorithms as shown in various publications (e.g., *Buchwitz et al., 2005; Butz et al., 2011; Frankenberg et al., 2011; Schneising et al., 2011; Parker et al., 2011; Scheper et al., 2012; Yoshida et al., 2013*). These products have been validated using Total Carbon Column Observing Network (TCCON) (*Wunch et al., 2010, 2011, 2015*) XCH_4 ground based observations (e.g., *Dils et al., 2014*).

In this document we describe the latest versions of these data products.

As an example, Figure 4 shows time series of satellite-derived XCH_4. As can be seen, XCH_4 is increasing since 2007 by about 7 ppb/year. The reason for this is not entirely clear (several potential reasons are discussed in the scientific literature).

Figure 4 – Satellite-derived northern mid-latitude XCH_4 time series. Shown are six time series, each corresponding to one of the four individual satellite sensor Level 2 XCH_4 products, which are described in this document.



1.1.5 List of XCO_2 and XCH_4 data products

Table 5 and Table 6 list the XCO_2 and XCH_4 data products, respectively.

As can be seen from Table 5, for each individual sensor Level 2 XCO_2 product two products have been generated using two different retrieval algorithms (OCFP is University of Leicester's Full Physics (FP) algorithm and SRFP is SRON's retrieval algorithm, also known as RemoTeC).

Products with comment « Existing GHG-CCI product » are the latest versions of Level 2 products, which have been generated in the framework of the ESA GHG-CCI project. They have been used within this C3S project to generate the merged Level 2 and Level 3 EMMA and OBS4MIPS products but the individual sensor L2 products have not been regenerated. They have been provided for C3S « as is » and are available via the C3S CDS.

Table 5 - Overview XCO_2 data products.

Product ID	Level	Sensor(s)	(Planned) Availability	Comments
CO2_GOS_OCFP	2	GOSAT	Oct. 2017: 2009-2016 Oct. 2018: 2009-2017 Dec. 2019: 2009-2018 Dec. 2020: 2009-2019	
CO2_GOS_SRFP	2	GOSAT	Oct. 2017: 2009-2016 Oct. 2018: 2009-2017 Dec. 2019: 2009-2018 Dec. 2020: 2009-2019	
CO2_SCI_BESD	2	SCIAMACHY	Oct. 2017: 2003-2012	Existing GHG-CCI product
CO2_SCI_WFMD	2	SCIAMACHY	Oct. 2017: 2002-2012	Existing GHG-CCI product
XCO2_EMMA	2	Merged SCIAMACHY, GOSAT, OCO-2	Oct. 2017: 2003-2016 Oct. 2018: 2003-2017 Dec. 2019: 2003-2018 Dec. 2020: 2003-2019	
XCO2_OBS4MIPS	3	Merged SCIAMACHY, GOSAT, OCO-2	Oct. 2017: 2003-2016 Oct. 2018: 2003-2017 Dec. 2019: 2003-2018 Dec. 2020: 2003-2019	

As can be seen from Table 6, for each individual sensor Level 2 XCH_4 product four products will be generated from GOSAT using four different retrieval algorithms using two « Full Physics » (FP) and two « Proxy » (PR) algorithms. For a discussion of FP versus PR algorithms see also, for example, *Schepers et al., 2012*. Each type of algorithm has different advantages and disadvantages. Typically, the PR products contain more data and therefore somewhat better spatio-temporal coverage (as quality filtering can be less strict) but the PR algorithms rely on a CO_2 model to correct for XCO_2 variations. FP products contain less data points but the advantage of this product is that it is independent of a CO_2 model.

Table 6 - Overview XCH_4 data products.

Product ID	Level	Sensor(s)	(Planned) Availability	Comments
CH4_GOS_OCPR	2	GOSAT	Oct. 2017: 2009-2016 Oct. 2018: 2009-2017 Dec. 2019: 2009-2018 Dec. 2020: 2009-2019	
CH4_GOS_SRPR	2	GOSAT	Oct. 2017: 2009-2016 Oct. 2018: 2009-2017 Dec. 2019: 2009-2018 Dec. 2020: 2009-2019	
CH4_GOS_OCFP	2	GOSAT	Oct. 2017: 2009-2016 Oct. 2018: 2009-2017 Dec. 2019: 2009-2018 Dec. 2020: 2009-2019	
CH4_GOS_SRFP	2	GOSAT	Oct. 2017: 2009-2016 Oct. 2018: 2009-2017 Dec. 2019: 2009-2018 Dec. 2020: 2009-2019	
CH4_SCI_WFMD	2	SCIAMACHY	Oct. 2017: 2002-2011	Existing GHG-CCI product
CH4_SCI_IMAP	2	SCIAMACHY	Oct. 2017: 2003-2012	Existing GHG-CCI product
XCH4_EMMA	2	Merged SCIAMACHY & GOSAT	Oct. 2017: 2003-2016 Oct. 2018: 2003-2017 Dec. 2019: 2003-2018 Dec. 2020: 2002-2019	
XCH4_OBS4MIPS	3	Merged SCIAMACHY & GOSAT	Oct. 2017: 2003-2016 Oct. 2018: 2003-2017 Dec. 2019: 2003-2018 Dec. 2020: 2003-2019	

1.2 Mid-tropospheric mixing ratios of CO_2 and CH_4

1.2.1 Overview

Satellite radiance observations in the thermal infrared (TIR) spectral region in nadir (downlooking) observation viewing mode are sensitive to atmospheric CO_2 and CH_4 mixing ratio changes in the mid and upper tropospheric region. They can thus be interpreted in terms of integrated mid-tropospheric columns, with typical sensitivity between 5 and 12 km.

In the following, the 2 hyperspectral infrared sounders AIRS and IASI are shortly described.

1.2.2 Instruments

1.2.2.1 AIRS

The Atmospheric Infrared Sounder (AIRS) is a polar orbiting nadir-viewing high-resolution infrared sounder operating in a cross-track-scanning mode. It was launched onboard the EOS Aqua satellite in May 2002, with two operational microwave sounders, AMSU and HSB, and is operational since September 2002. It is a high-spectral resolution, grating multispectral infrared sounder with 2378 channels. Its spectral domain ranges from 650 cm^{-1} to 2665 cm^{-1} (15.4 µm and 3.8 µm), with a spectral resolving power of 1200 (i.e., a spectral resolution ranging from 0.5 cm^{-1} to 2 cm^{-1}). This domain is divided into three spectral bands, from 650 to 1135 cm^{-1}, from 1215 to 1615 cm^{-1} and from 2180 to 2665 cm^{-1}. AIRS cross-track scanning is 1650 km and covers 70% of the earth every day. The instantaneous field of view (IFOV) is sampled by 3×3 circular pixels whose ground resolution is 13 km at nadir. Measurements from the three instruments are analyzed jointly to filter out the effects of clouds from the IR data in order to derive clear-column air-temperature profiles and surface temperatures with high vertical resolution and accuracy (1 K per 1 km layer in the troposphere).

1.2.2.2 IASI

The Infrared Atmospheric Sounding Interferometer (IASI) is a high resolution Fourier Transform Spectrometer based on a Michelson Interferometer coupled to an integrated imaging system that measures infrared radiation emitted from the Earth. Developed by the Center National d'Etudes Spatiales (CNES) in collaboration with the European Organisation for the Exploitation of Meteorological Satellites (EUMETSAT), IASI was launched in October 2006 onboard the polar orbiting Meteorological Operational Platform (Metop-A), and in September 2012 onboard Metop-B. A third IASI will be launched onboard Metop-C. IASI provides 8461 spectral samples, ranging from 645 cm^{-1} to 2760 cm^{-1} (15.5 µm and 3.6 µm), with a spectral sampling of 0.25 cm^{-1}, and a spectral resolution of 0.5 cm^{-1} after apodisation ('Level 1c' spectra). IASI is an across track scanning system, whose swath width is of 2200 km, allowing global coverage twice a day. The IFOV is sampled by 2×2 circular pixels whose ground resolution is 12 km at nadir. IASI has demonstrated the possibility to retrieve or detect several chemistry and climate variables from hyperspectral infrared observation: for instance water vapour (H_2O), carbon dioxide (CO_2), carbon monoxide (CO), methane (CH_4), ozone (O_3), sulfur dioxide (SO_2), hydrogen sulfide (H_2S), ammonia (NH_3), nitric acid (HNO_3), volatile organic compounds (VOCs) and aerosols (*Hilton et al., 2012; Clarisse et al., 2011*) on regional and global scales. IASI enables the monitoring of key gases for climate and atmospheric chemistry in near real time and has also highlighted the benefit of high-performance infrared sounders for numerical weather prevision (NWP) applications.

1.2.3 CO_2

Mid-tropospheric columns of CO_2 can be retrieved from hyperspectral infrared sounders such as AIRS and IASI (*Chédin et al., 2003; Crevoisier et al., 2003*) using non-linear inference scheme (Crevoisier et al., 2009a).

Products have been validated using aircraft measurements, mostly from the Comprehensive Observation Network for TRace gases by AIrLiner (CONTRAIL) program (*Machida et al., 2008; Matsueda et al. 2008*).

1.2.4 CH_4

Mid-tropospheric columns of CH_4 can be retrieved from the hyperspectral infrared sounder IASI (Crevoisier et al., 2003, 2013) using non-linear inference scheme (*Crevoisier et al., 2009b*).

Products have been validated using aircraft measurements, from the Comprehensive Observation Network for TRace gases by AIrLiner (CONTRAIL) program (*Machida et al., 2008; Matsueda et al. 2008*) and the HIAPER Pole-to-Pole Observations (HIPPO) project (Wofsy et al., 2012), as well as from balloon measurements from AirCores (*Membrive et al., 2016*).

1.2.5 List of mid-tropospheric CO_2 and CH_4 data products

Table 7 lists the CO_2 and CH_4 mid/upper troposphere data products.

The product with comment « Existing GHG-CCI product » is the latest versions of AIRS CO_2 Level 2 products, which has been generated in the framework of the ESA GHG-CCI project. It has been provided for C3S essentially « as is » but converted (from ASCII) to NetCDF format (all products listed in Table 7 are available in NetCDF format).

Table 7 - Overview mid/upper troposphere CO_2 and CH_4 data products.

Product ID	Level	Sensor(s)	(Planned) Availability	Comments
CO2_IASA_NLIS	2	IASI / Metop-A	Oct. 2017: 2007-2015 Dec. 2020: 2007-2019	
CH4_IASA_NLIS	2	IASI / Metop-A	Oct. 2017: 2007-2015 Dec. 2020: 2007-2019	
CO2_IASB_NLIS	2	IASI / Metop-B	Oct. 2017: 2013-2016 Oct. 2018: 2013-2017 Dec. 2019: 2013-2018 Dec. 2020: 2013-2019	
CH4_IASB_NLIS	2	IASI / Metop-B	Oct. 2017: 2013-2016 Oct. 2018: 2013-2017 Dec. 2019: 2013-2018 Dec. 2020: 2013-2019	
CO2_AIR_NLIS	2	AIRS	Feb. 2017: 2003-2007	Existing GHG-CCI product

2. Product validation methodology

2.1 Description of reference data used for validation

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

2.1.1.1 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 limitation as explained in Sect. 2.2.1.4.1.

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 20 TCCON sites (see Sect. 2.2.1.4.1).

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. 2.2.1.1.

2.1.1.2 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.

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

2.1.2.1 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 onboard commercial airliners: CONTRAIL, IAGOS in the future.
- aircraft regular measurements made by research groups: NOAA aircraft network in the US and Canada.
- aircraft research campaigns: HIPPO, CoMet in the future.
- Balloon measurements: AirCores at various locations (Timmins, Kiruna, Sodankulä, Trainou-Orléans).

2.1.2.2 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.

2.2 Description of product validation methodology

2.2.1 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.

2.2.1.1 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., B*uchwitz 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.

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. Overall 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.

2.2.1.2 Methods to be applied to the C3S ECV CDR data set

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.

2.2.1.2.1 Quantitative assessment methods

For each data product the following quantities have been determined:

<u>Single ground pixel random error (or “single measurement precision”, 1-sigma):</u>
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.

<u>Reported uncertainties (“Uncertainty ratio”):</u>
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 observations. 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. See also document PVIRv5 (*Buchwitz et al., 2017*) for an assessment of this quantity using the pre-cursor products.

<u>Mean bias:</u>
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 (see data quality summary Figure 1 for XCO_2 and Figure 2 for XCH_4), where the results from all assessment methods are presented. 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. Also the 1-sigma uncertainty needs to be reported as obtain 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.

2.2.1.2.2 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 about the entire data set.
- Comparisons with global models (in particular those assimilating accurate surface CO_2 and CH_4 measurements).

2.2.1.3 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 need to be 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

<u>(Relative) Accuracy:</u>

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. 2.2.1.2.1) 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 enhanced 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:

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

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 5 for XCO_2 and Figure 6 for XCH_4.

Figure 5 - Probability that the XCO_2 accuracy TR is met as a function of the achieved accuracy.

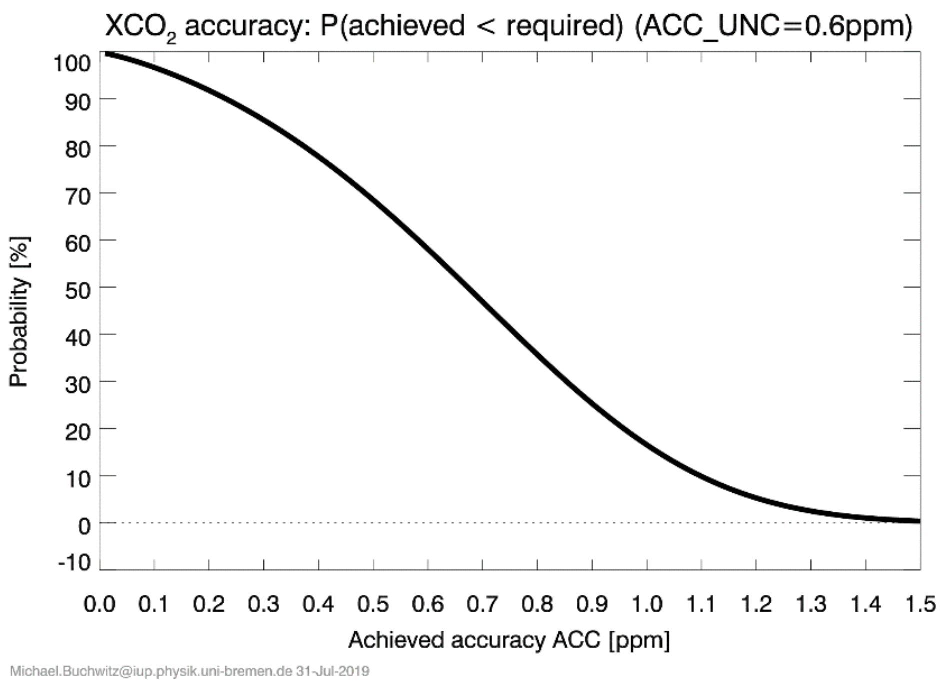
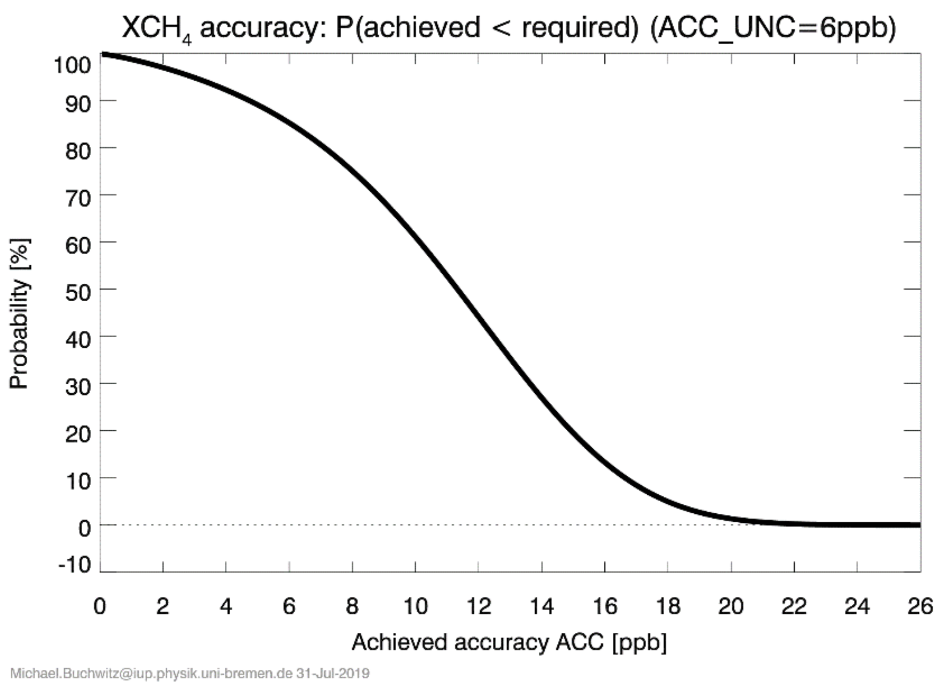


Figure 6 - Probability that the XCH_4 accuracy TR is met as a function of the achieved accuracy.



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).

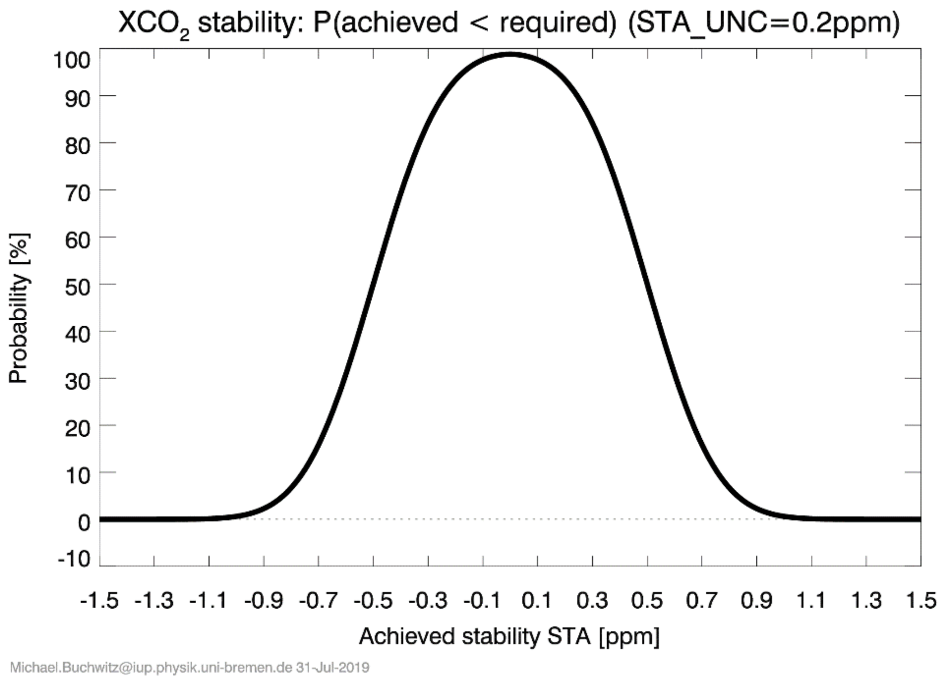
Quadratically adding the assumed TCCON uncertainty gives for this example for STA +/- UNC_STA:

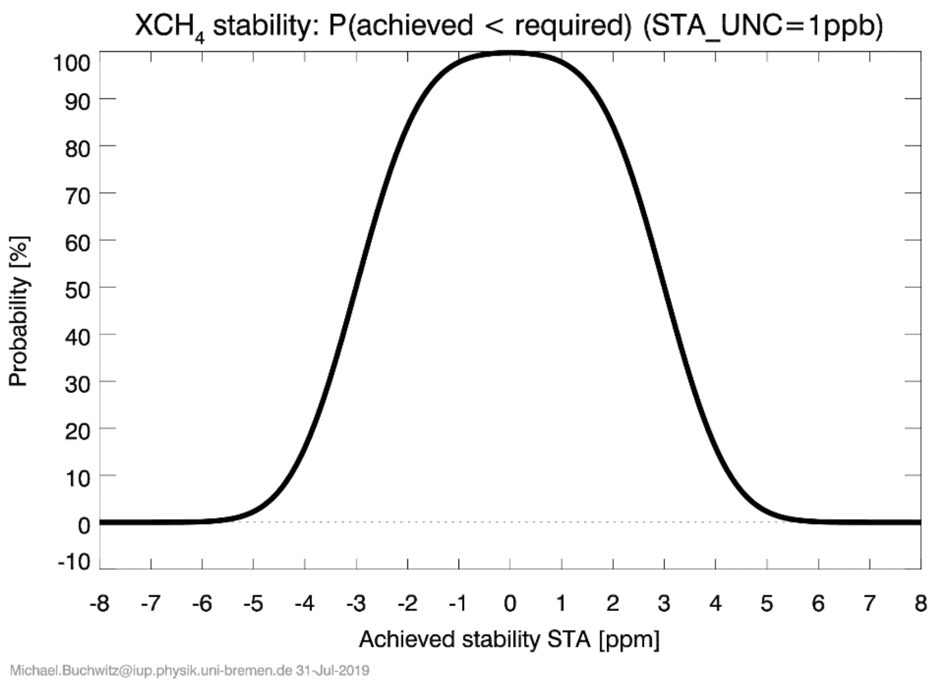
- XCO_2: +0.1 +/- 0.21 (1-sigma) ppm/year
- XCH_4: -0.8 +/- 1.08 (1-sigma) ppb/year

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 7 shows how the used probability functions look like.

Figure 7 – Probability functions used to obtain the probability that the stability requirement is met. Top: for XCO_2. Bottom: for XCH_4.



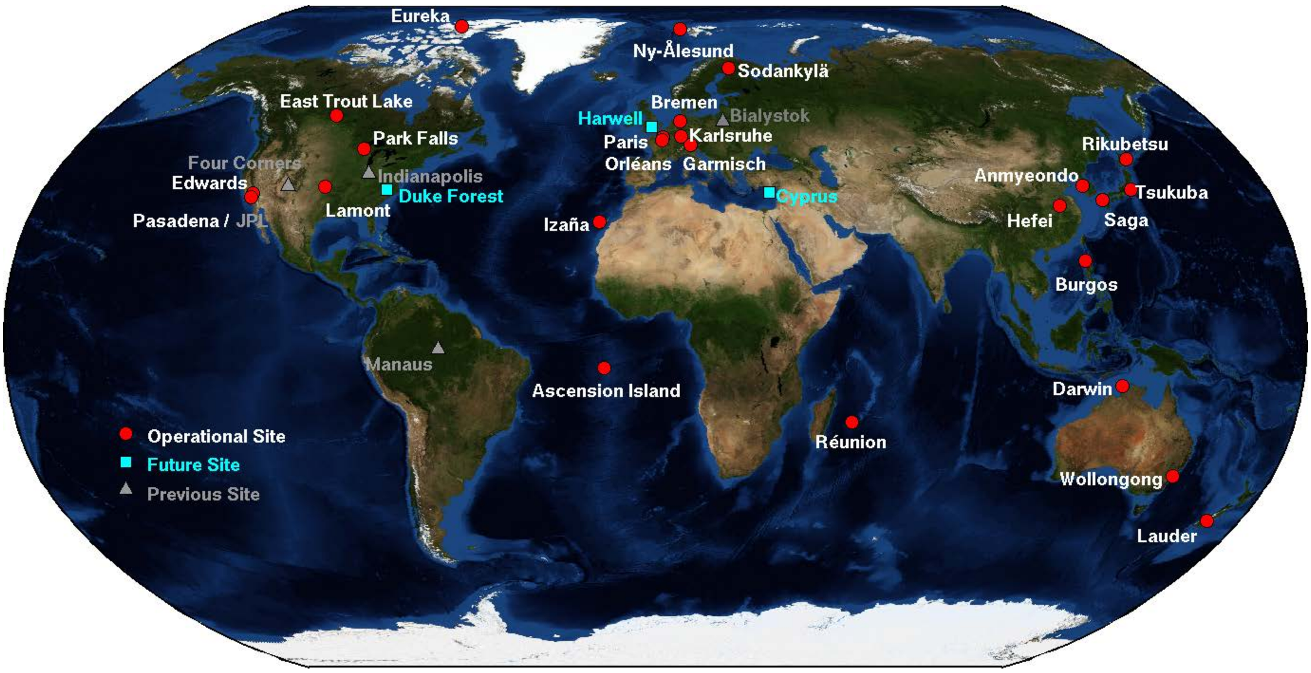


2.2.1.4 Known limitations

2.2.1.4.1 TCCON

The TCCON network consists of about 20 TCCON sites (see Figure 8). 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 8 - Location of TCCON sites. Source: http://www.tccon.caltech.edu/.



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

It would therefore be highly beneficial for this service

- if the TCCON network would be 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 would be available faster (current availability: one year after observation).
- if the quality of the TCCON retrievals would be further improved (if possible) as the current data quality (approx. 0.4 ppm for XCO_2 (1-sigma) and 4 ppb for XCH_4 (1-sigma)) is on the order of the required data quality of the satellite retrievals.

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

2.2.2 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.

They have been generated such that the products likely get approval from the Obs4MIPs committee (https://www.earthsystemcog.org/projects/obs4mips/). The C3S Obs4MIPs products are updates of pre-cursor products generated in the framework of ESA's GHG-CCI project.

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. Nevertheless, quality assessments similar as for the Level 2 products have been carried out including TR assessments.

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

2.2.3.1 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 will be extended for C3S in the context of the C3S_312a_Lot6 project.

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 enable 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.

2.2.3.2 Methods applied to the C3S ECV CDR data set

2.2.3.2.1 Quantitative assessment methods

Essentially the same methods have been applied as described in Sect. 2.2.1.2.1 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.

2.2.3.2.2 Qualitative assessment methods

The same methods have been applied as described in Sect. 2.2.1.2.2 for the XCO_2 and XCH_4 data products.

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

Essentially the same methods have been applied as described in Sect. 2.2.1.2.1 for the XCO_2 and XCH_4 data products.

2.2.3.4 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.

3. Validation results

3.1 Validation results for Level 2 XCO_2 products

In this section, the validation method as explained in the previous section is applied to the XCO_2 and XCH_4 Level 2 individual sensor pre-cursor products, which have been generated in the framework of the ESA project GHG-CCI (*Buchwitz et al., 2016*). The main purpose of this section is to illustrate the method and to show which data quality can be expected from the to be generated C3S XCO_2 and XCH_4 Level 2 data products. The used products are from the latest GHG-CCI data set called "Climate Research Data Package No. 4" (CRDP4, see *Buchwitz et al., 2017*).

For each data product a set of well defined "figures of merit" (FoMs) need to be computed to summarize the validation results and to compute the probability that the TR is met as explained in Sect. 2.2. This can be done using different methods 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).

In the following sub-sections results from one of the methods are presented. This method is a method developed and implemented at Univ. Bremen for the validation of all C3S XCO_2 and XCH_4 Level 2 data products. For the final validation also other methods will be used, in particular the methods applied by each data provider to validate their own data set(s). 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*).

The validation results as shown in this document are based on the TCCON products from 22 TCCON sites: Eureka, NyAlesund, Sodankyla, East Trout Lake, Bialystok, Bremen, Karlsruhe, Paris, Orleans, Garmisch, Park Falls, Lamont, Tsukuba, Edwards, Caltech, Saga, Burgos, Ascension Island, Darwin, Reunion Island, Wollongong, Lauder- Detailed information on each site can be found at https://tccon-wiki.caltech.edu/Sites. The used TCCON version is GGG2014 (data access: 27-May-2019).

Co-location criteria:

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

3.1.1 Validation results for product CO2_SCI_BESD

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 9 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 9 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 10** for product CO2_SCI_BESD. The top right part shows a table listing the FoMs as obtained for the individual TCCON sites (the Lamont (LAM) results are shown in **Figure 9**). 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 9) and
- FoMs characterising stability in terms of drift and year-to-year bias variability (see caption Figure 9 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_SCI_BESD product, which are listed in the yellow marked box in the bottom right of **Figure 10**:

- 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. 2.2.1.3 for details).

These final FoMs are used for **Table 8**, which summarizes the quality assessment results for this product.

Figure 9 - Comparison of satellite XCO_2 product CO2_SCI_BESD (red symbols in top panel) with TCCON XCO_2 (black symbols in top panel). 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 numbers are listed at the bottom (reported as mean value and standard deviation) using the same colors 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).

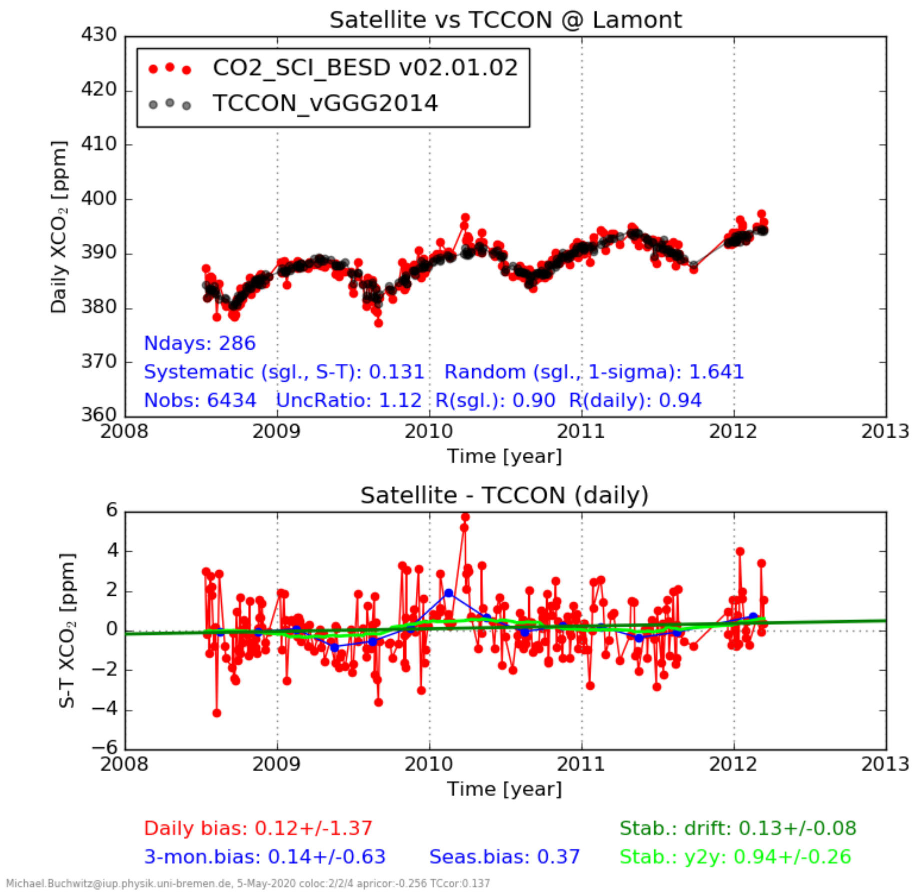


Figure 10 - Product Quality Summary Figure for product CO2_SCI_BESD. Please see the main text for a detailed explanation.

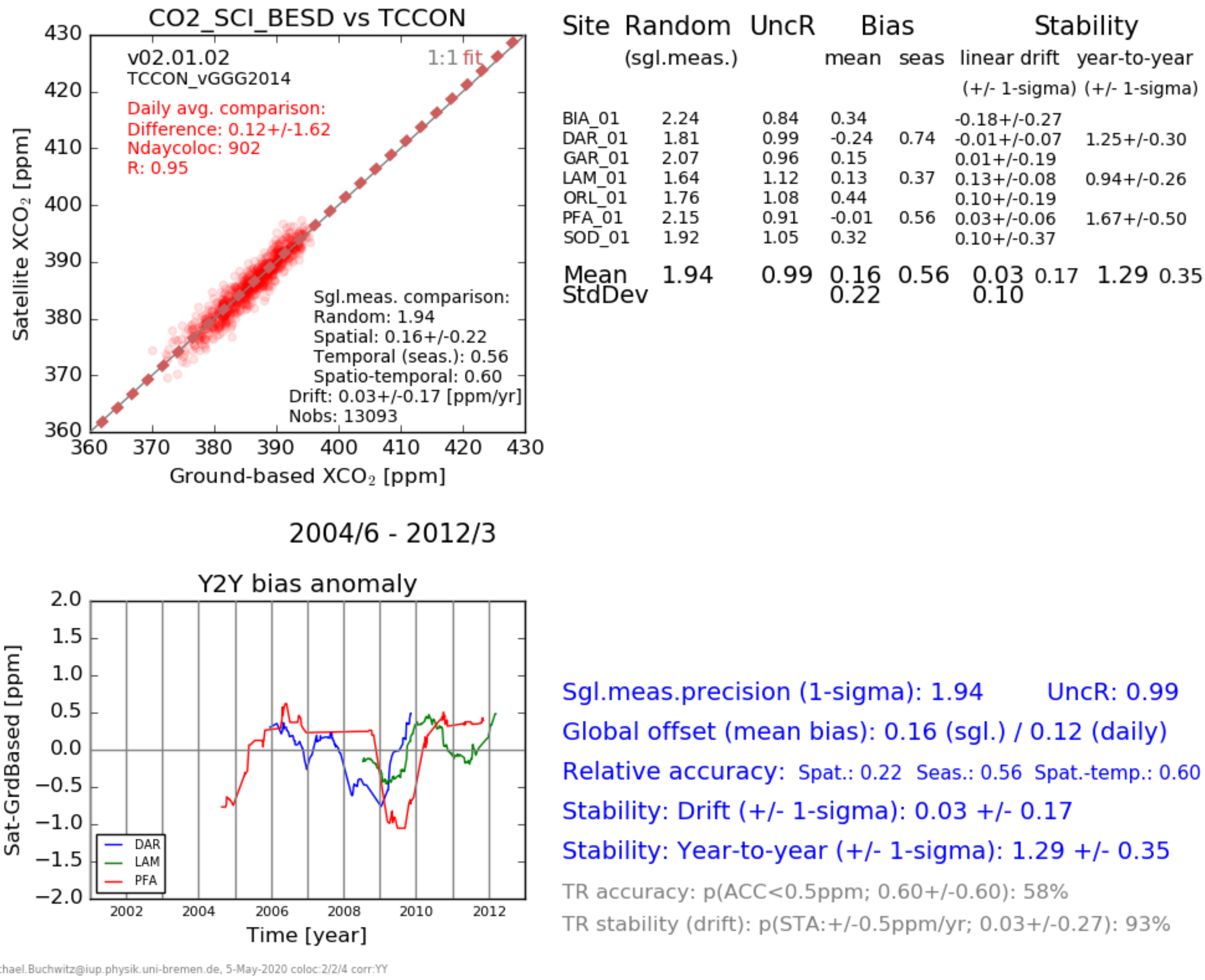


Table 8 - Product Quality Summary Table for product CO2_SCI_BESD as obtained by comparison with TCCON reference data using the QA/QC assessment method. The listed requirements are the threshold (T) requirements as given in *TRD (D4)*. For precision (i.e., single observation statistical uncertainty or 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_SCI_BESD Level: 2, Version: 02.01.02, Time period covered: 1.2003 – 3.2012				
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	0.99	-	-	No requirement but value close to unity expected for a high quality data product.
Mean bias [ppm]	0.16	-	-	No requirement but value close to zero expected for a high quality data product.
Accuracy: Relative systematic error [ppm]	Spatial – spatiotemporal: 0.22 – 0.60	< 0.5	Probability that accuracy TR is met: 58%	-
Stability: Drift [ppm/year]	0.03 +/- 0.17 (1-sigma)	< 0.5	Probability that stability TR is met: 93%	-
Stability: Year-to-year bias variability [ppm/year]	1.3 +/- 0.4 (1-sigma)	< 0.5	-	-

3.1.2 Validation results for product CO2_SCI_WFMD

Similar figures as shown in 3.1.1 for product CO2_SCI_BESD are shown in this section but for product CO2_SCI_WFMD.

The Product Quality Summary Table for product CO2_SCI_WFMD is shown as Table 9.

Figure 11 - As Figure 9 but for product CO2_SCI_WFMD.

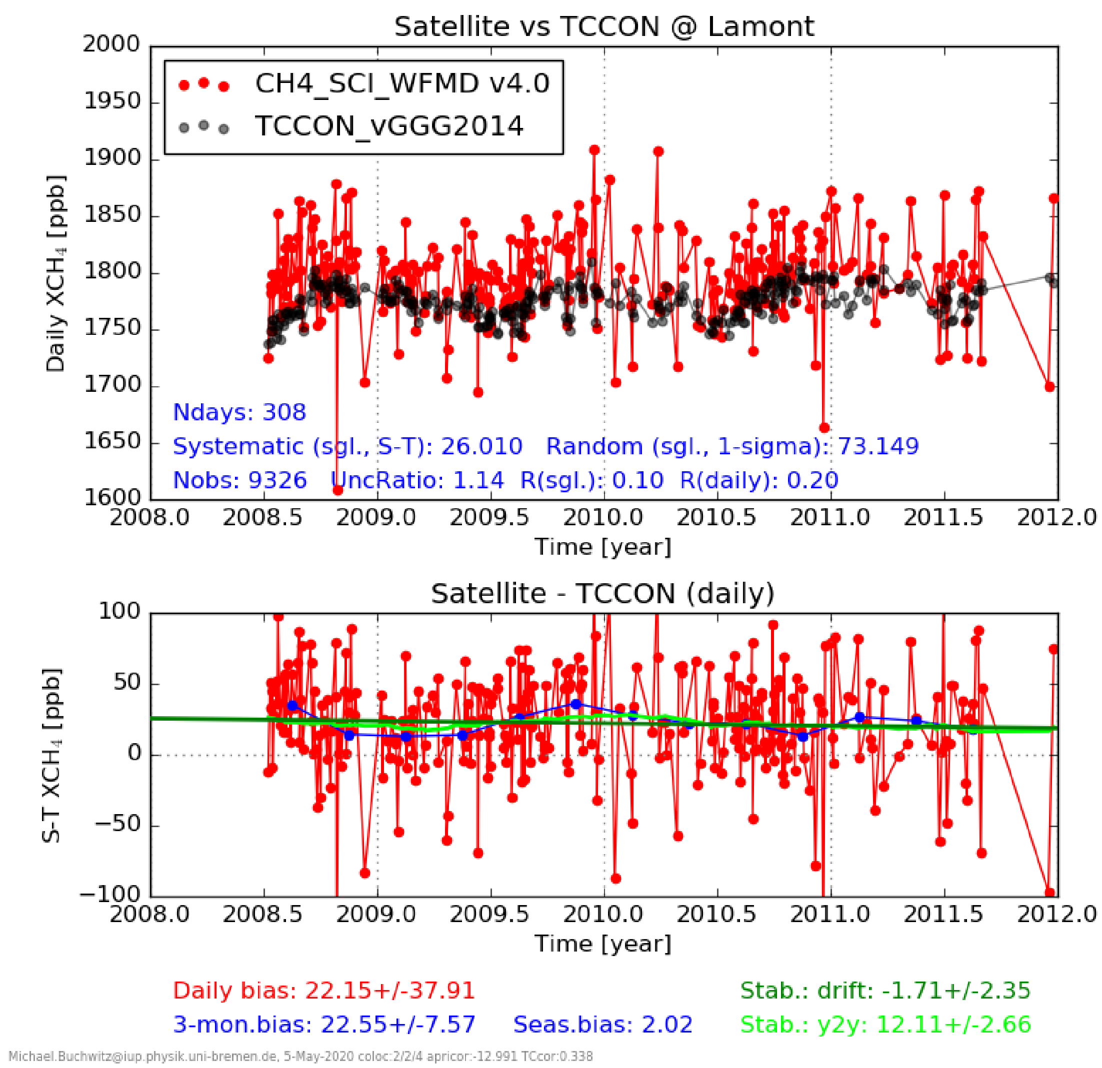


Figure 12 - As **Figure 10** but for product CO2_SCI_WFMD.

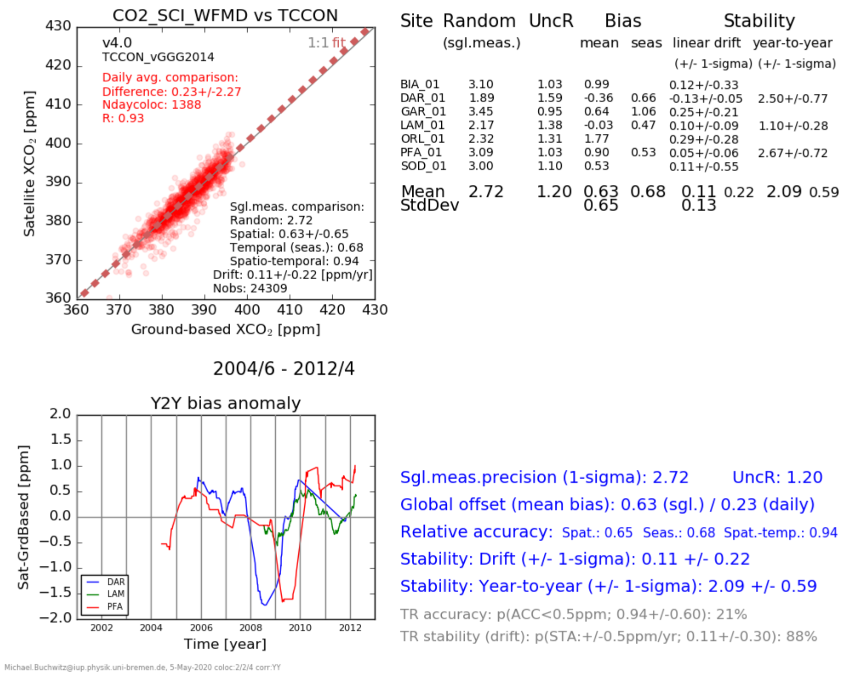


Table 9 - Product Quality Summary Table for product CO2_SCI_WFMD.

Product Quality Summary Table for Product: CO2_SCI_WFMD Level: 2, Version: 4.0, Time period covered: 10.2002 – 4.2012				
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	1.20	-	-	No requirement but value close to unity expected for a high quality data product.
Mean bias [ppm]	0.63	-	-	No requirement but value close to zero expected for a high quality data product.
Accuracy: Relative systematic error [ppm]	Spatial – spatiotemporal: 0.65 – 0.94	< 0.5	Probability that accuracy TR is met: 21%	-
Stability: Drift [ppm/year]	0.11 +/- 0.22 (1-sigma)	< 0.5	Probability that stability TR is met: 88%	-
Stability: Year-to-year bias variability [ppm/year]	2.1 +/- 0.6 (1-sigma)	< 0.5	-	-

3.1.3 Validation results for product CO2_GOS_OCFP

Similar figures as shown in 3.1.1 for product CO2_SCI_BESD are shown in this section but for product CO2_GOS_OCFP.

The Product Quality Summary Table for product CO2_GOS_OCFP is shown as Table 9.

Figure 13 - As Figure 9 but for product CO2_GOS_OCFP.

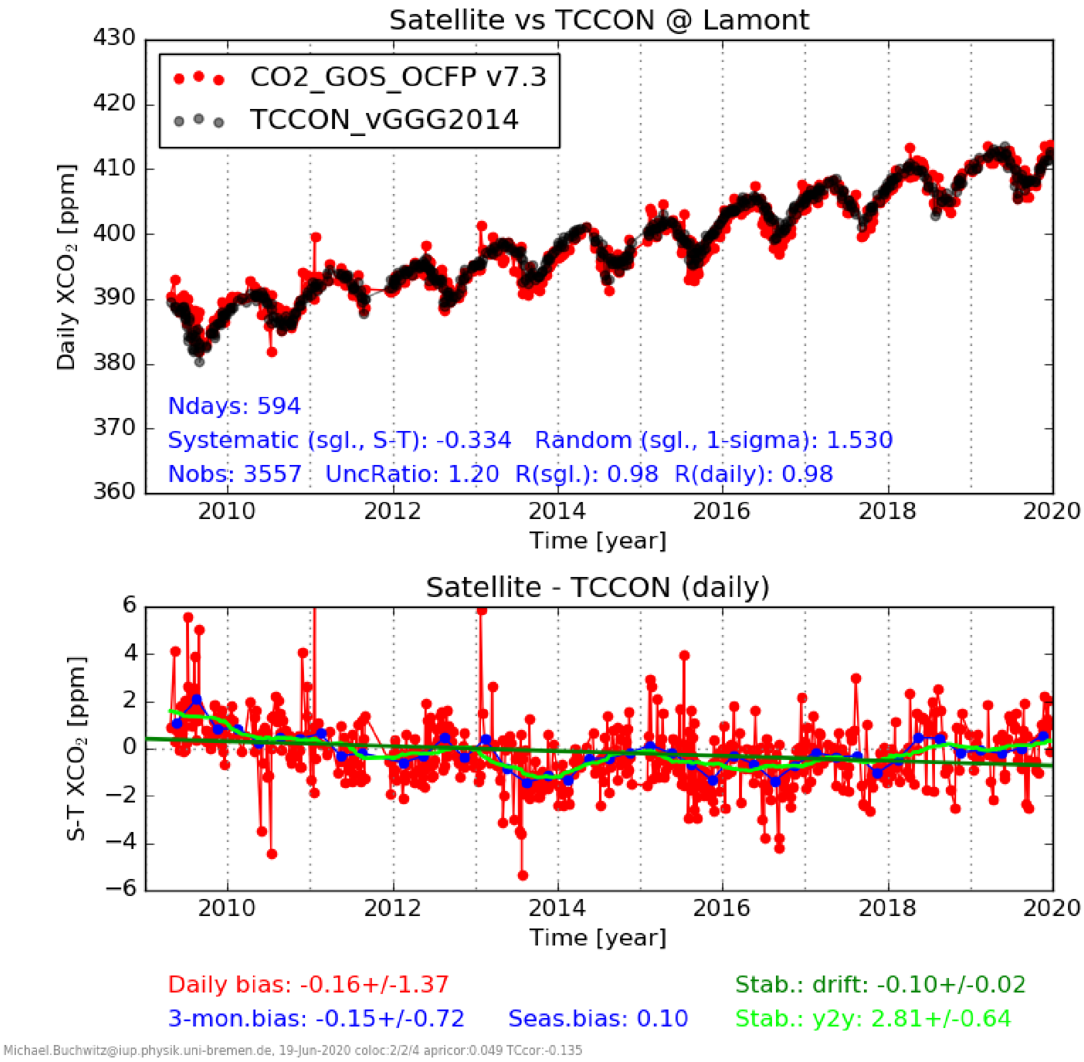


Figure 14 - As **Figure 10** but for product CO2_GOS_OCFP.

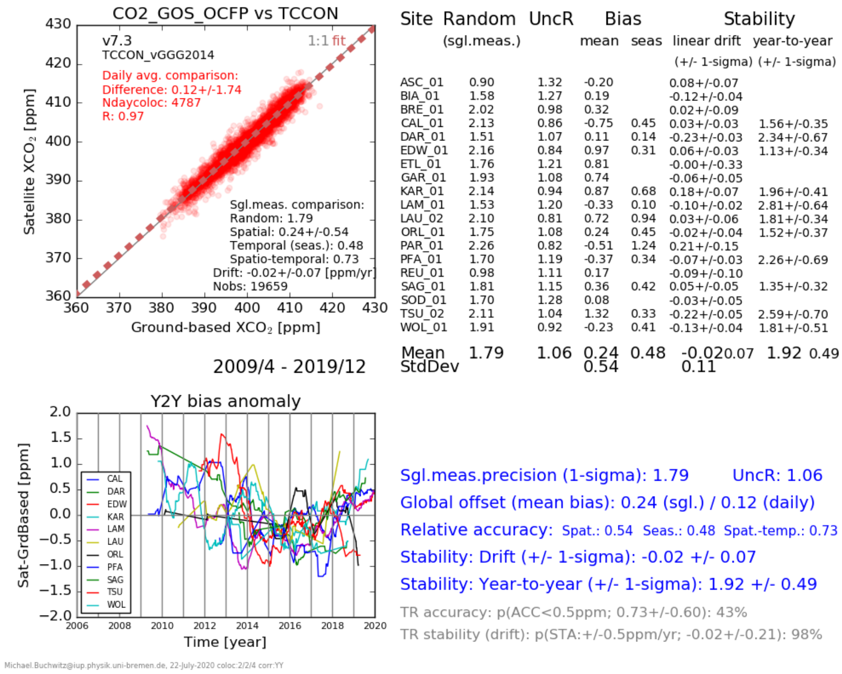


Table 10 - Product Quality Summary Table for product CO2_GOS_OCFP.

Product Quality Summary Table for Product: CO2_GOS_OCFP Level: 2, Version: 7.3, Time period covered: 4.2009 – 12.2019				
Parameter [unit]	Achieved performance	Requirement	TR	Comments
Single measurement precision (1-sigma) in [ppm]	1.8	< 8 (T) < 3 (B) < 1 (G)	-	-
Uncertainty ratio) in [-]: Ratio reported uncertainty to standard deviation of satellite-TCCON difference	1.06	-	-	No requirement but value close to unity expected for a high quality data product.
Mean bias [ppm]	0.24	-	-	No requirement but value close to zero expected for a high quality data product.
Accuracy: Relative systematic error [ppm]	Spatial – spatiotemporal: 0.54 – 0.73	< 0.5	Probability that accuracy TR is met: 43%	-
Stability: Drift [ppm/year]	-0.02 +/- 0.07 (1-sigma)	< 0.5	Probability that stability TR is met: 98%	-
Stability: Year-to-year bias variability [ppm/year]	1.9 +/- 0.5 (1-sigma)	< 0.5	-	-

3.1.4 Validation results for product CO2_GOS_SRFP

Similar figures as shown in 3.1.1 for product CO2_SCI_BESD 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 11.

Figure 15 - As Figure 9 but for product CO2_GOS_SRFP.

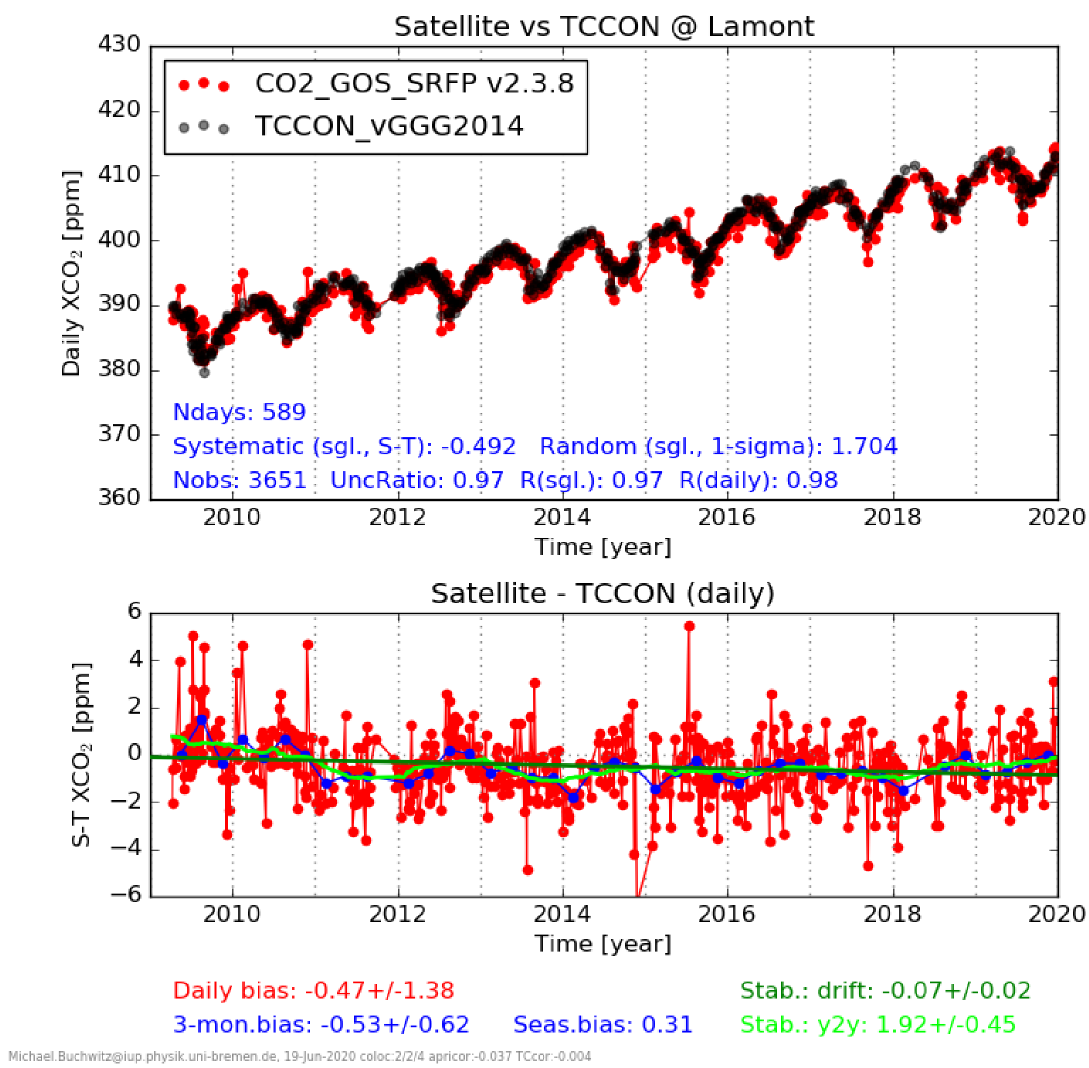


Figure 16 – As **Figure 10** but for product CO2_GOS_SRFP.

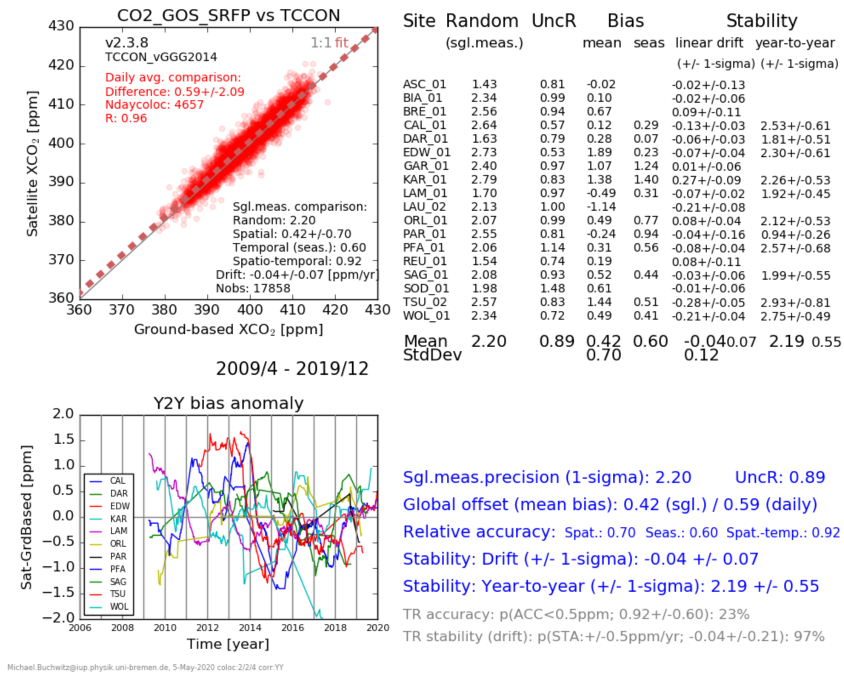


Table 11 - Product Quality Summary Table for product CO2_GOS_SRFP.

Product Quality Summary Table for Product: CO2_GOS_SRFP Level: 2, Version: 2.3.8, Time period covered: 4.2009 – 12.2019				
Parameter [unit]	Achieved performance	Requirement	TR	Comments
Single measurement precision (1-sigma) in [ppm]	2.2	< 8 (T) < 3 (B) < 1 (G)	-	-
Uncertainty ratio) in [-]: Ratio reported uncertainty to standard deviation of satellite-TCCON difference	0.89	-	-	No requirement but value close to unity expected for a high quality data product.
Mean bias [ppm]	0.42	-	-	No requirement but value close to zero expected for a high quality data product.
Accuracy: Relative systematic error [ppm]	Spatial – spatiotemporal: 0.70 – 0.92	< 0.5	Probability that accuracy TR is met: 23%	-
Stability: Drift [ppm/year]	-0.04 +/- 0.07 (1-sigma)	< 0.5	Probability that stability TR is met: 97%	-
Stability: Year-to-year bias variability [ppm/year]	2.2 +/- 0.6 (1-sigma)	< 0.5	-	-

3.1.5 Validation results for product XCO2_EMMA

Similar figures as shown in 3.1.1 for product CO2_SCI_BESD are shown in this section but for product XCO2_EMMA.

The Product Quality Summary Table for product XCO2_EMMA is shown as Table 11.

Figure 17 - As Figure 9 but for product XCO2_EMMA.

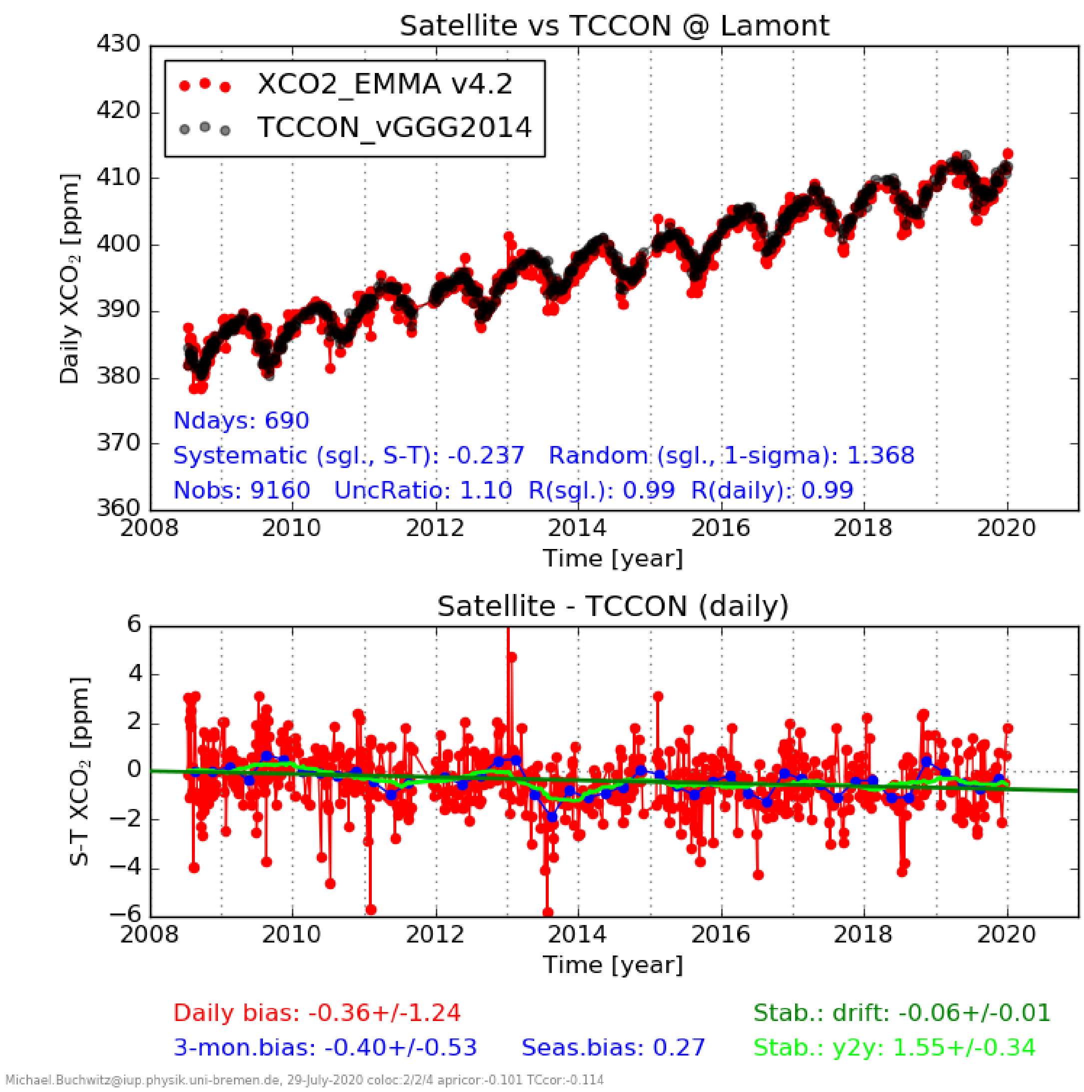


Figure 18 - As **Figure 10** but for product XCO2_EMMA.

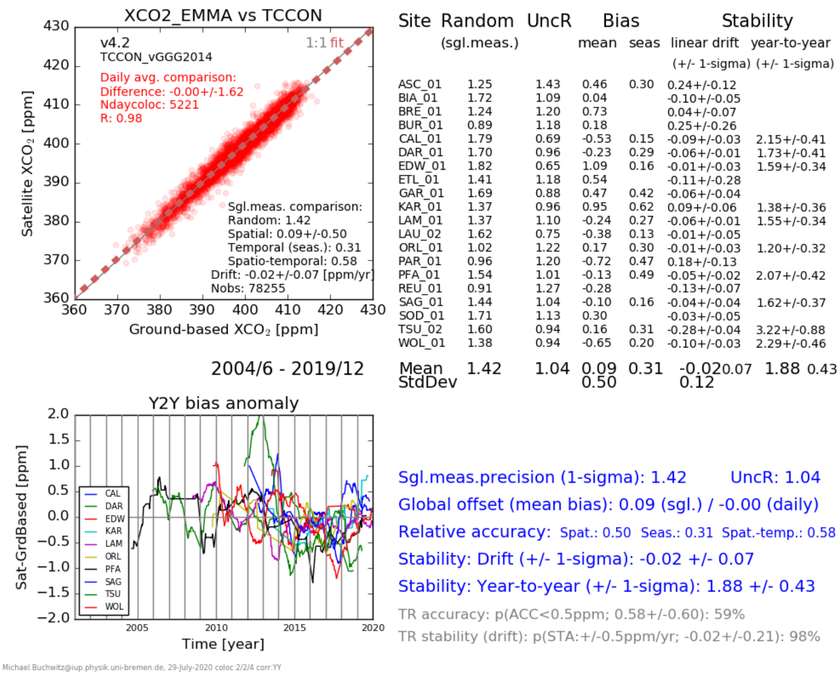


Table 12 - Product Quality Summary Table for product XCO2_EMMA.

Product Quality Summary Table for Product: XCO2_EMMA Level: 2, Version: 4.2, Time period covered: 1.2003 – 12.2019				
Parameter [unit]	Achieved performance	Requirement	TR	Comments
Single measurement precision (1-sigma) in [ppm]	1.42	< 8 (T) < 3 (B) < 1 (G)	-	-
Uncertainty ratio) in [-]: Ratio reported uncertainty to standard deviation of satellite-TCCON difference	1.04	-	-	No requirement but value close to unity expected for a high quality data product.
Mean bias [ppm]	0.09	-	-	No requirement but value close to zero expected for a high quality data product.
Accuracy: Relative systematic error [ppm]	Spatial – spatiotemporal: 0.50 – 0.58	< 0.5	Probability that accuracy TR is met: 59%	-
Stability: Drift [ppm/year]	-0.02 +/- 0.07 (1-sigma)	< 0.5	Probability that stability TR is met: 98%	-
Stability: Year-to-year bias variability [ppm/year]	1.88 +/- 0.43 (1-sigma)	< 0.5	-	-

3.2 Validation results of Level 2 XCH_4 products

In this section the validation method as explained in the previous section is applied to the XCO_2 and XCH_4 Level 2 individual sensor pre-cursor products, which have been generated in the framework of the ESA project GHG-CCI (*Buchwitz et al., 2016*). The main purpose of this section is to illustrate the method and to show which data quality can be expected from the to be generated C3S XCO_2 and XCH_4 Level 2 data products. The used products are from the latest GHG-CCI data set called "Climate Research Data Package No. 4" (CRDP4, see *Buchwitz et al., 2017*).

For each data product a set of well defined "figures of merit" (FoMs) need to be computed to summarize the validation results and to compute the probability that the TR is met as explained in Sect. 2.2. This can be done using different methods 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).

In the following sub-sections results from one of the methods are presented. This method is a method developed and implemented at Univ. Bremen for the validation of all C3S XCO_2 and XCH_4 Level 2 data products. For the final validation also other methods will be used, in particular the methods applied by each data provider to validate their own data set(s). 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*).

The validation results as shown in this document are based on the TCCON products from 22 TCCON sites: Eureka, NyAlesund, Sodankyla, East Trout Lake, Bialystok, Bremen, Karlsruhe, Paris, Orleans, Garmisch, Park Falls, Lamont, Tsukuba, Edwards, Caltech, Saga, Burgos, Ascension Island, Darwin, Reunion Island, Wollongong, Lauder- Detailed information on each site can be found at https://tccon-wiki.caltech.edu/Sites. The used TCCON version is GGG2014 (data access: 27-May-2019).

Co-location criteria:

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

3.2.1 Validation results for product CH4_SCI_WFMD

Similar figures as shown in 3.1.1 for product CO2_SCI_BESD are shown in this section but for product CH4_SCI_WFMD.

The Product Quality Summary Table for product CH4_SCI_WFMD is shown as Table 13.

Figure 19 - As Figure 9 but for product CH4_SCI_WFMD.

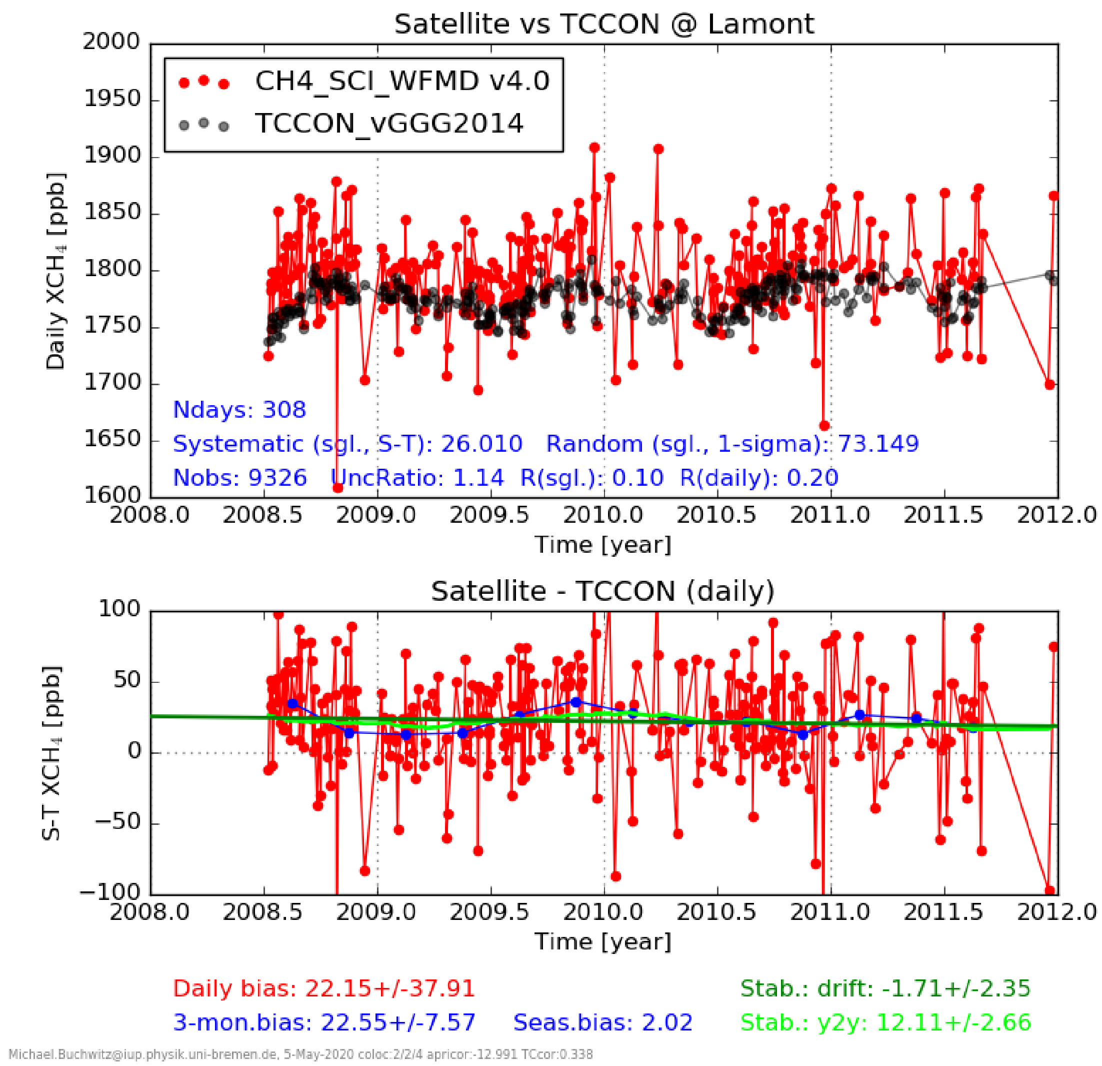


Figure 20 - As **Figure 10** but for product CH4_SCI_WFMD.

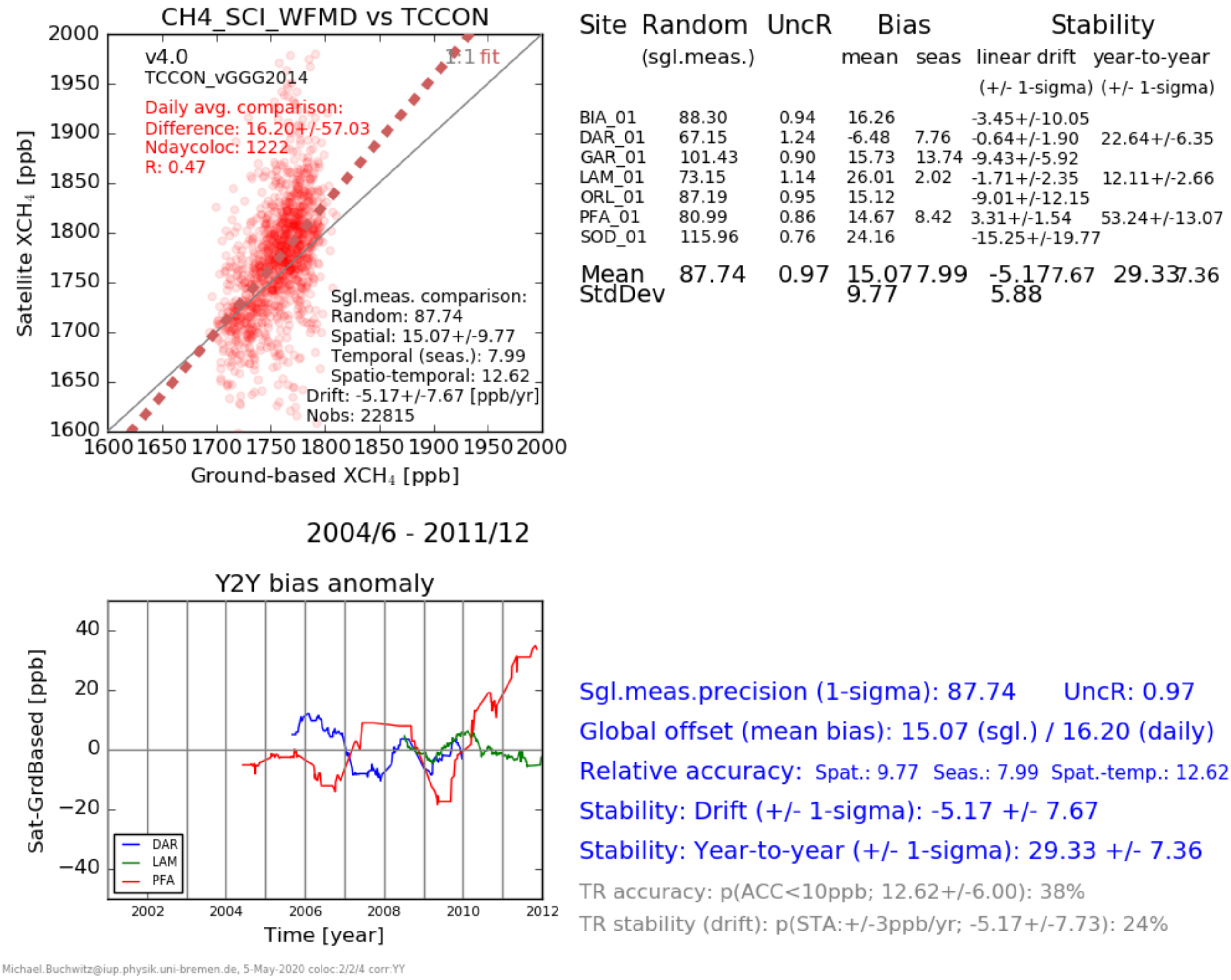


Table 13 - Product Quality Summary Table for product CH4_SCI_WFMB as obtained by comparison with TCCON reference data. The listed requirements are the threshold (T) requirements as given in *TRD (D4)*. For precision (i.e., single observation statistical uncertainty or random error) also the corresponding breakthrough (B) and goal (G) requirements are listed. For the achieved performance of "Accuracy" two values are listed: The first one is the spatial component of the bias (computed as the standard deviation of the bias as the TCCON sites), the second one is the temporal (seasonal) component of the bias. The probability that the accuracy TR is met is computed using the largest of the two accuracy values.

Product Quality Summary Table for Product: CH4_SCI_WFMD Level: 2, Version: 4.0, Time period covered: 10.2002 – 12.2011				
Parameter [unit]	Achieved performance	Requirement	TR	Comments
Single measurement precision (1-sigma) in [ppb]	88	< 34 (T) < 17 (B) < 9 (G)	-	-
Uncertainty ratio) in [-]: Ratio reported uncertainty to standard deviation of satellite-TCCON difference	0.97	-	-	No requirement but value close to unity expected for a high quality data product.
Mean bias [ppb]	15.1	-	-	No requirement but value close to zero expected for a high quality data product.
Accuracy: Relative systematic error [ppb]	Spatial – spatiotemporal: 10 – 13	< 10	Probability that accuracy TR is met: 38%	-
Stability: Linear bias trend [ppb/year]	-5 +/- 8 (1-sigma)	< 3	Probability that stability TR is met: 24%	-
Stability: Year-to-year bias variability [ppb/year]	29 +/- 7 (1-sigma)	< 3	-	-

3.2.2 Validation results for product CH4_SCI_IMAP

Similar figures as shown in 3.1.1 for product CO2_SCI_BESD are shown in this section but for product CH4_SCI_IMAP.

The Product Quality Summary Table for product CH4_SCI_IMAP is shown as Table 14.

Figure 21 - As Figure 9 but for product CH4_SCI_IMAP.

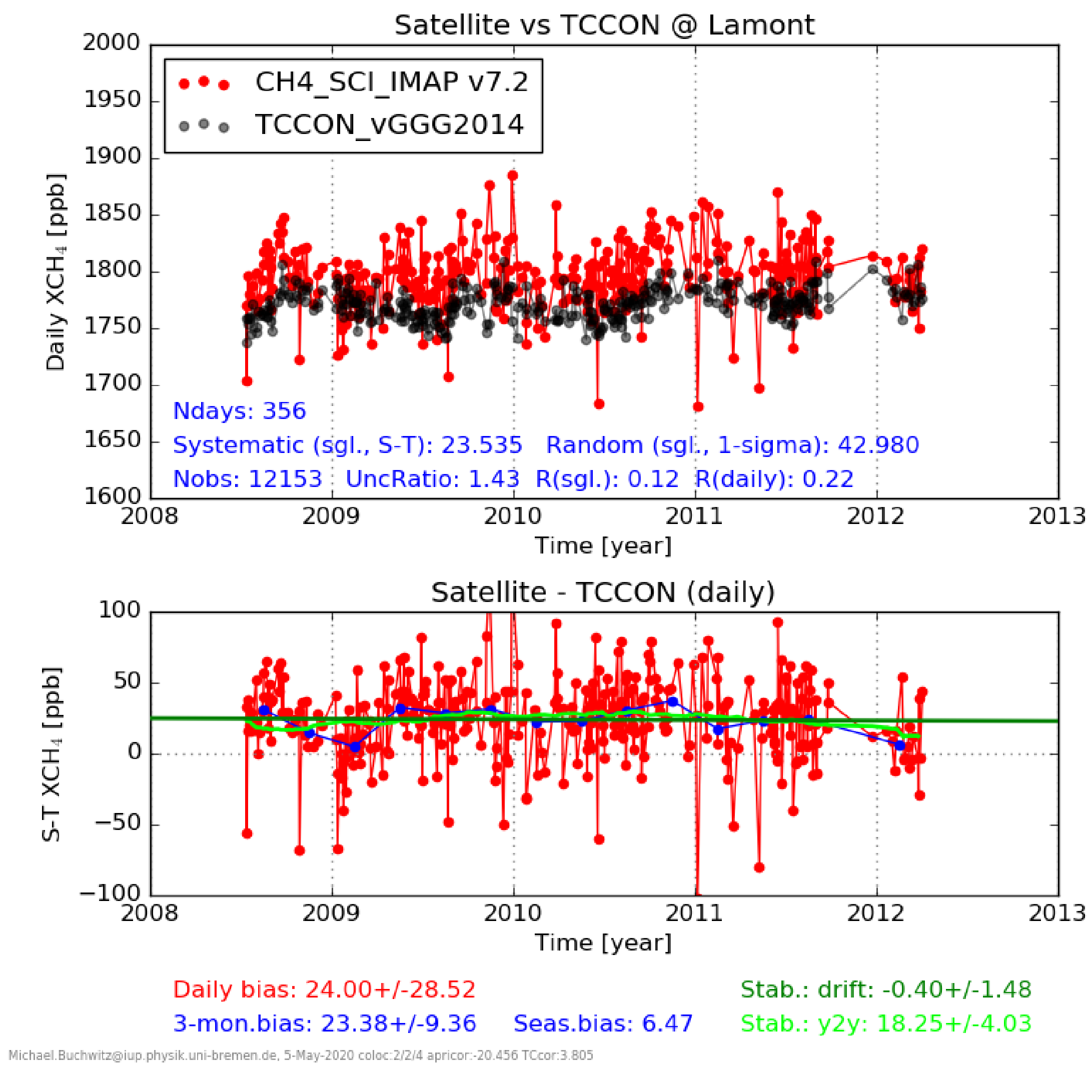


Figure 22 - As **Figure 10** but for product CH4_SCI_IMAP.

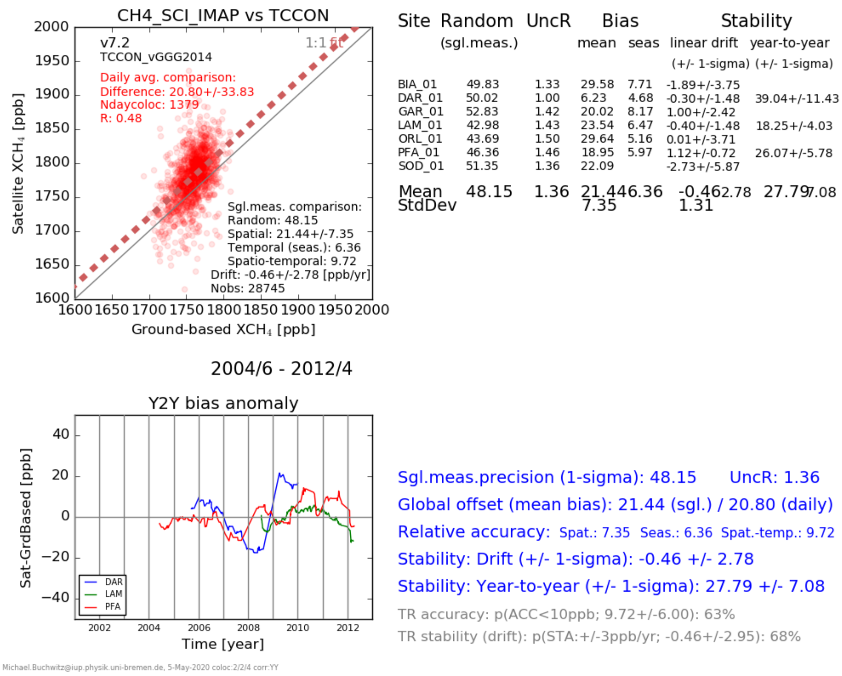


Table 14 - Product Quality Summary Table for product CH4_SCI_IMAP.

Product Quality Summary Table for Product: CH4_SCI_IMAP Level: 2, Version: 7.2, Time period covered: 1.2003 – 4.2012				
Parameter [unit]	Achieved performance	Requirement	TR	Comments
Single measurement precision (1-sigma) in [ppb]	48	< 34 (T) < 17 (B) < 9 (G)	-	-
Uncertainty ratio) in [-]: Ratio reported uncertainty to standard deviation of satellite-TCCON difference	1.36	-	-	No requirement but value close to unity expected for a high quality data product.
Mean bias [ppb]	21.4	-	-	No requirement but value close to zero expected for a high quality data product.
Accuracy: Relative systematic error [ppb]	Spatial – spatiotemporal: 7.4 – 9.8	< 10	Probability that accuracy TR is met: 63%	-
Stability: Linear bias trend [ppb/year]	-0.5 +/- 2.8 (1-sigma)	< 3	Probability that stability TR is met: 68%	-
Stability: Year-to-year bias variability [ppb/year]	28 +/- 7 (1-sigma)	< 3	-	-

3.2.3 Validation results for product CH4_GOS_OCPR

Similar figures as shown in 3.1.1 for product CO2_SCI_BESD 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 15.

Figure 23 - As Figure 9 but for product CH4_GOS_OCPR.

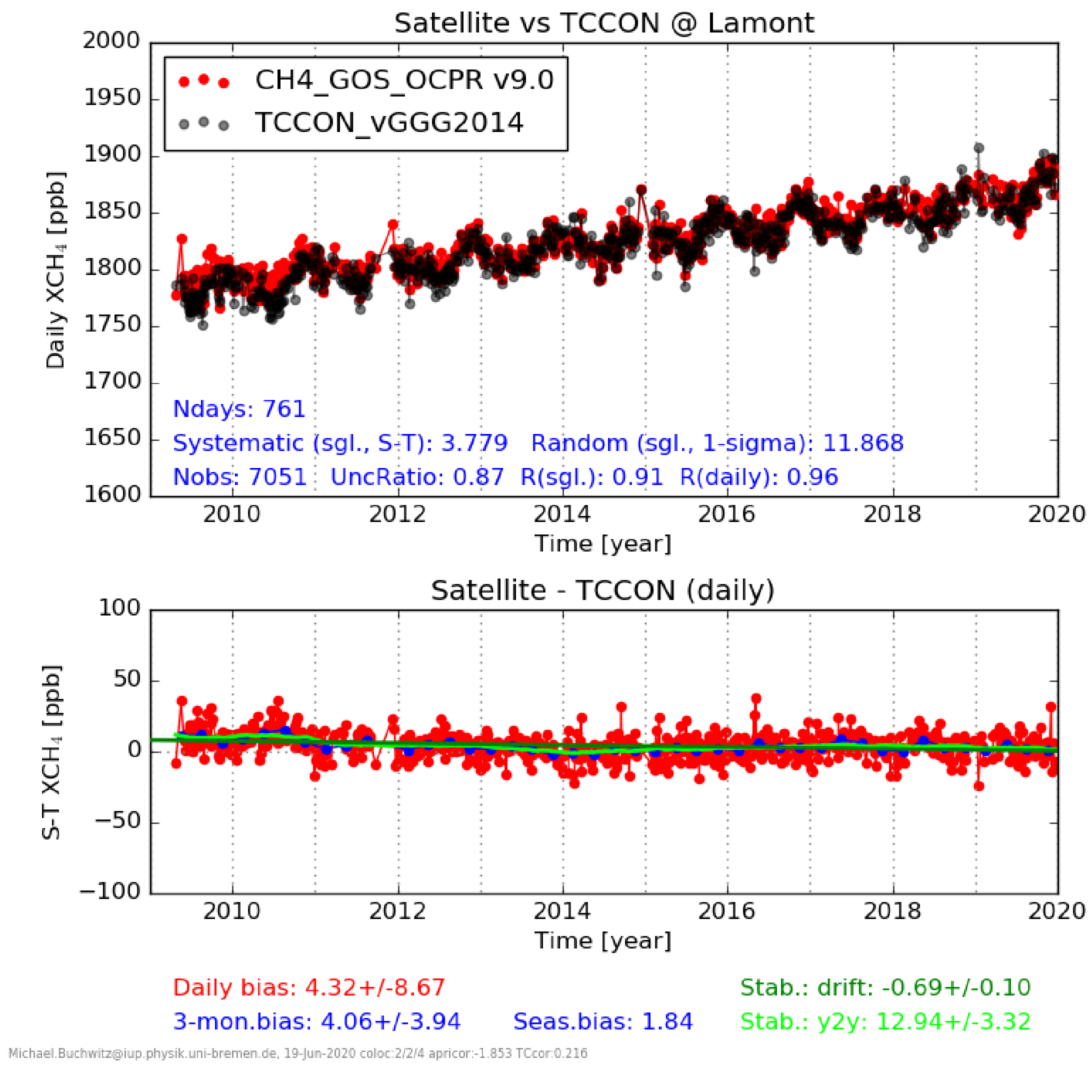


Figure 24 - As **Figure 10** but for product CH4_GOS_OCPR.

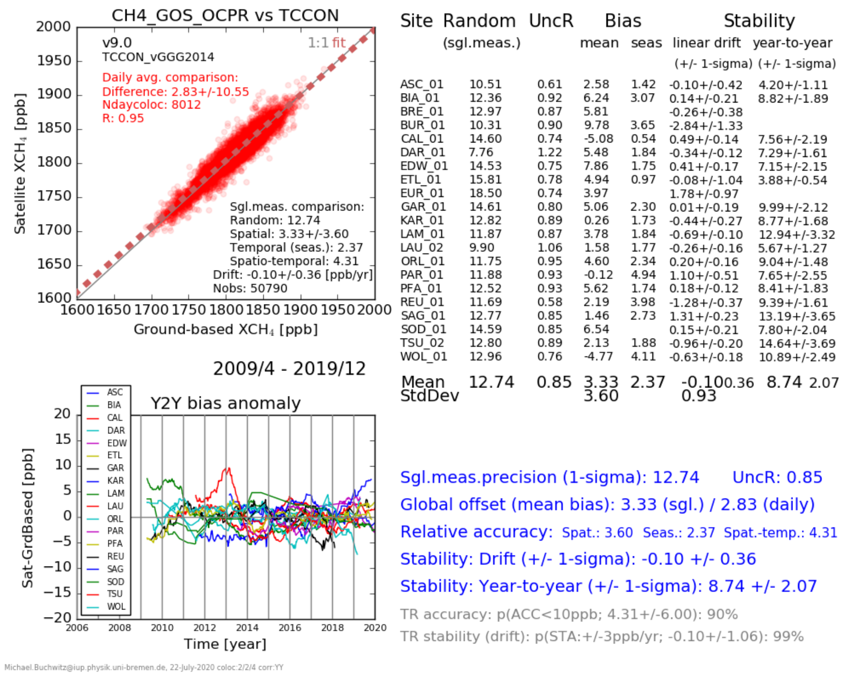


Table 15 - Product Quality Summary Table for product CH4_GOS_OCPR.

Product Quality Summary Table for Product: CH4_GOS_OCPR Level: 2, Version: 9.0, Time period covered: 4.2009 – 12.2019				
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	0.85	-	-	No requirement but value close to unity expected for a high quality data product.
Mean bias [ppb]	3.3	-	-	No requirement but value close to zero expected for a high quality data product.
Accuracy: Relative systematic error [ppb]	Spatial – spatiotemporal: 3.6 – 4.3	< 10	Probability that accuracy TR is met: 90%	-
Stability: Linear bias trend [ppb/year]	-0.1 +/- 0.4 (1-sigma)	< 3	Probability that stability TR is met: 99%	-
Stability: Year-to-year bias variability [ppb/year]	9 +/- 2 (1-sigma)	< 3	-	-

3.2.4 Validation results for product CH4_GOS_SRPR

Similar figures as shown in 3.1.1 for product CO2_SCI_BESD are shown in this section but for product CH4_GOS_SRPR.

The Product Quality Summary Table for product CH4_GOS_SRPR is shown as Table 16.

Figure 25 - As Figure 9 but for product CH4_GOS_SRPR.

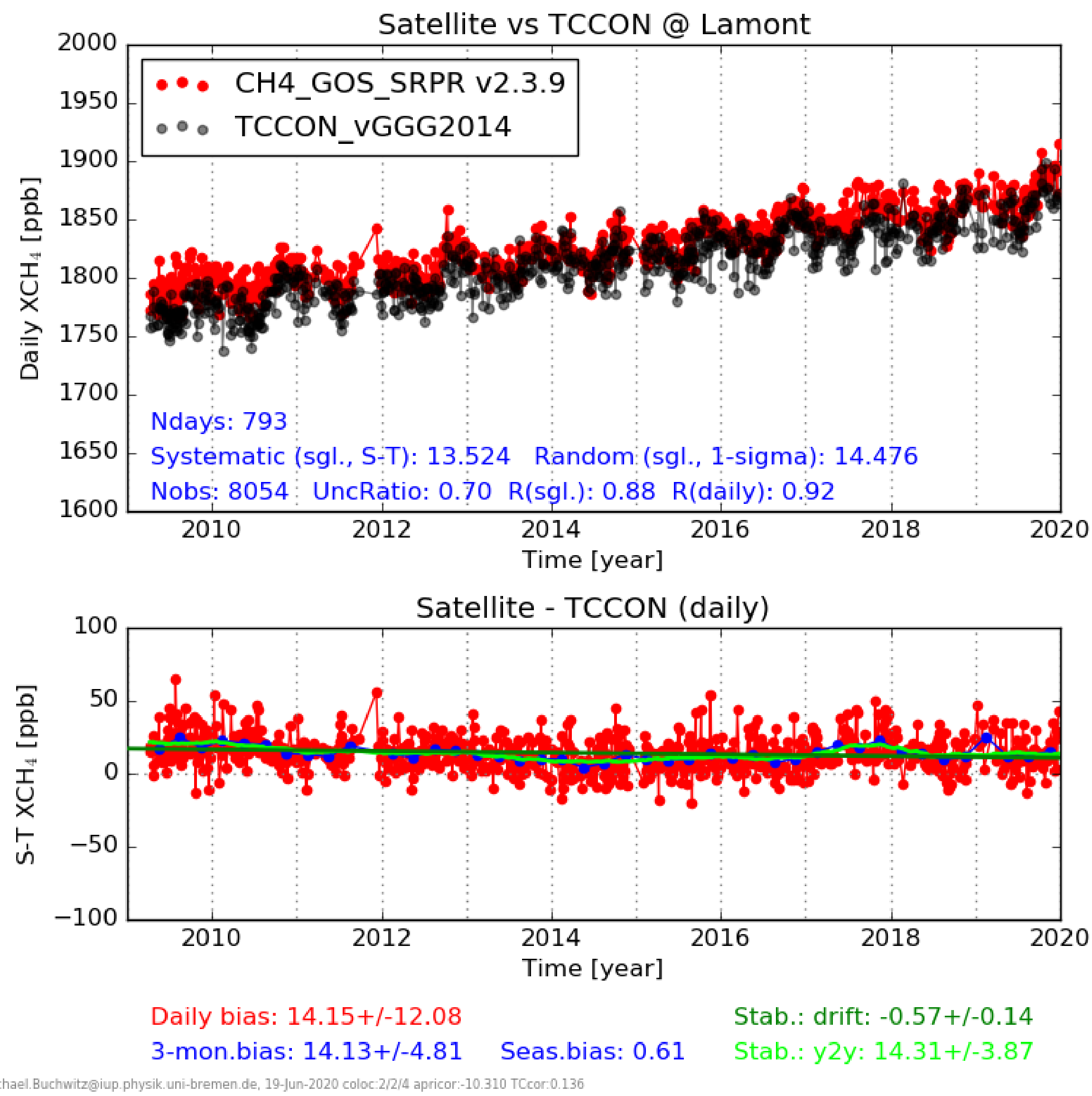


Figure 26 - As **Figure 10** but for product CH4_GOS_SRPR.

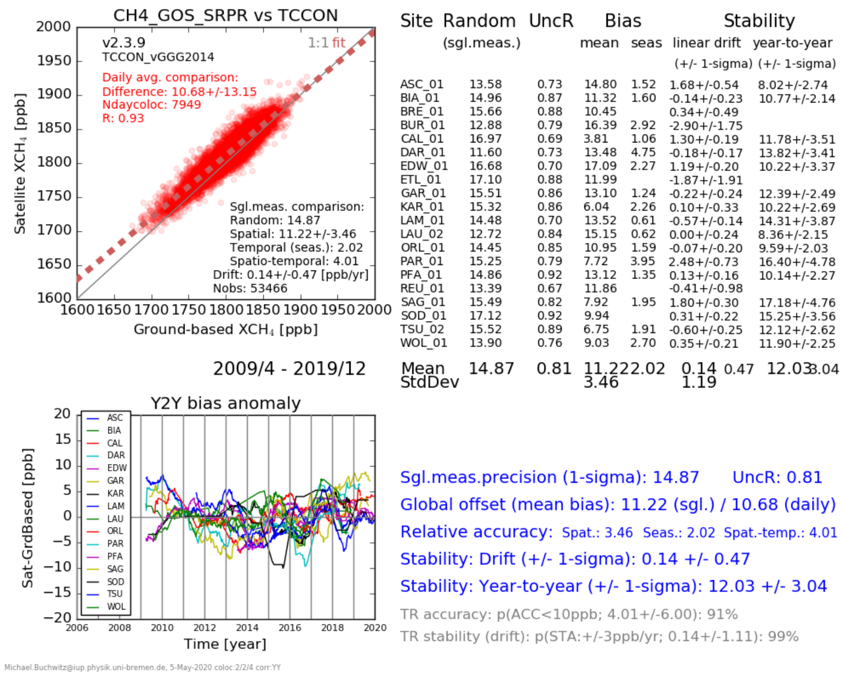


Table 16 - Product Quality Summary Table for product CH4_GOS_SRPR.

Product Quality Summary Table for Product: CH4_GOS_SRPR Level: 2, Version: 2.3.9, Time period covered: 4.2009 – 12.2019				
Parameter [unit]	**Achieved performance**	**Requirement**	**TR**	**Comments**
Single measurement precision (1-sigma) in [ppb]	14.9	< 34 (T) < 17 (B) < 9 (G)	-	-
Uncertainty ratio) in [-]: Ratio reported uncertainty to standard deviation of satellite-TCCON difference	0.81	-	-	No requirement but value close to unity expected for a high quality data product.
Mean bias [ppb]	11.2	-	-	No requirement but value close to zero expected for a high quality data product.
Accuracy: Relative systematic error [ppb]	Spatial – spatiotemporal: 3.5 – 4.0	< 10	Probability that accuracy TR is met: 91%	-
Stability: Linear bias trend [ppb/year]	0.14 +/- 0.47 (1-sigma)	< 3	Probability that stability TR is met: 99%	-
Stability: Year-to-year bias variability [ppb/year]	12 +/- 3 (1-sigma)	< 3	-	-

3.2.5 Validation results for product CH4_GOS_OCFP

Similar figures as shown in 3.1.1 for product CO2_SCI_BESD 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 17.

Figure 27 - As Figure 9 but for product CH4_GOS_OCFP.

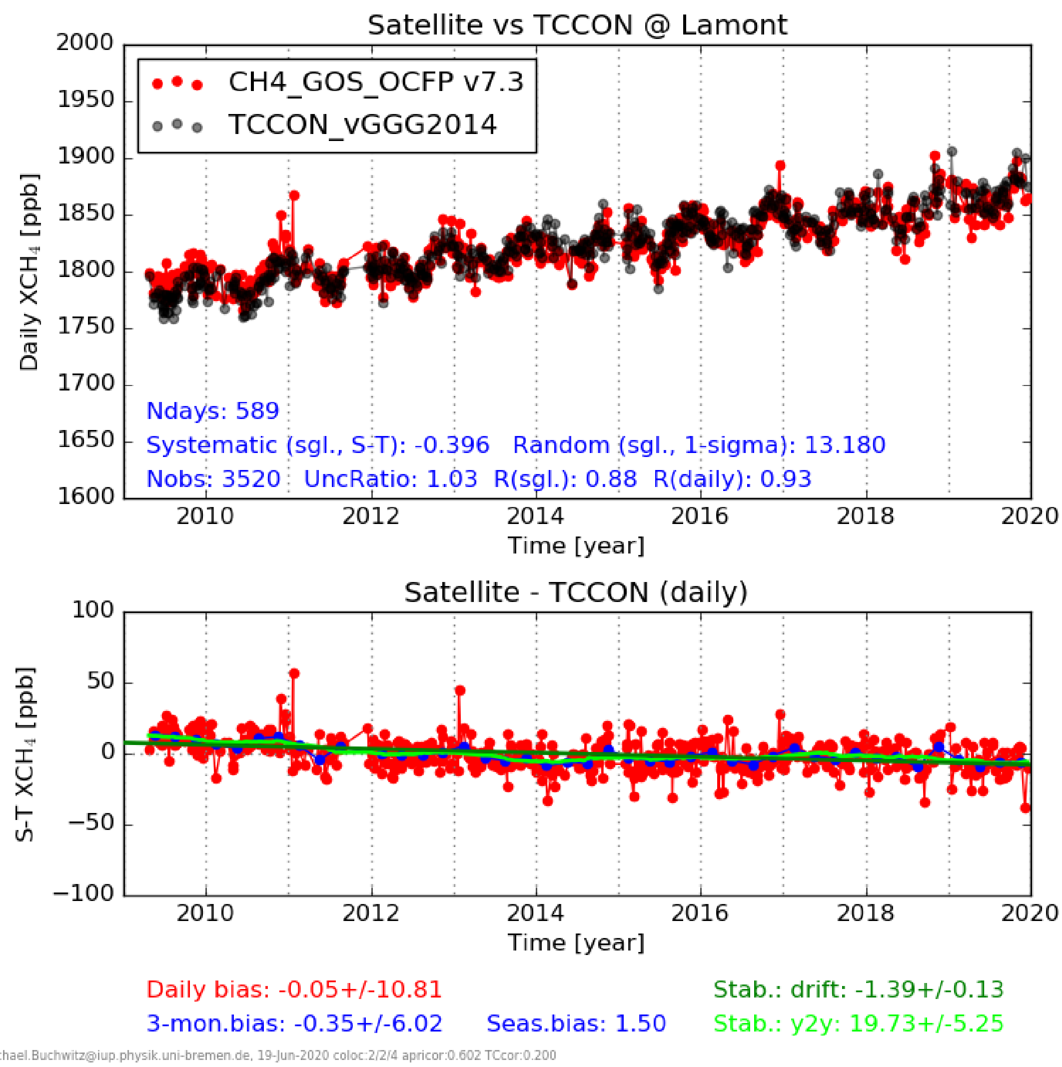


Figure 28 - As **Figure 10** but for product CH4_GOS_OCFP.

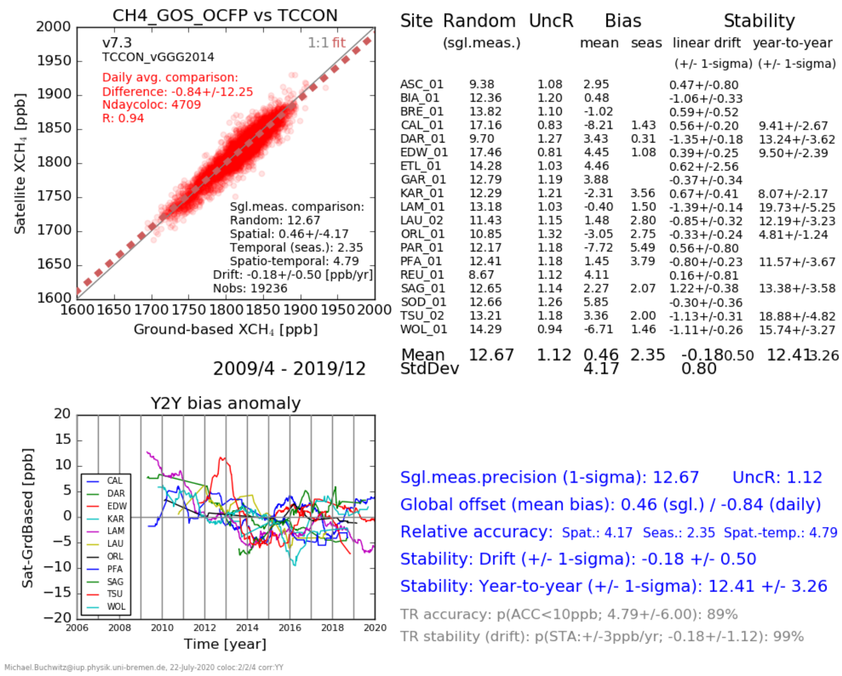


Table 17 - Product Quality Summary Table for product CH4_GOS_OCFP.

Product Quality Summary Table for Product: CH4_GOS_OCFP Level: 2, Version: 7.3, Time period covered: 4.2009 – 12.2019				
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	1.12	-	-	No requirement but value close to unity expected for a high quality data product.
Mean bias [ppb]	0.46	-	-	No requirement but value close to zero expected for a high quality data product.
Accuracy: Relative systematic error [ppb]	Spatial – spatiotemporal: 4.2 – 4.8	< 10	Probability that accuracy TR is met: 89%	-
Stability: Linear bias trend [ppb/year]	-0.2 +/- 0.5 (1-sigma)	< 3	Probability that stability TR is met: 99%	-
Stability: Year-to-year bias variability [ppb/year]	12 +/- 3 (1-sigma)	< 3	-	-

3.2.6 Validation results for product CH4_GOS_SRFP

Similar figures as shown in 3.1.1 for product CO2_SCI_BESD are shown in this section but for product CH4_GOS_OCFP.

The Product Quality Summary Table for product CH4_GOS_SRFP is shown as Table 18.

Figure 29 - As Figure 9 but for product CH4_GOS_SRFP.

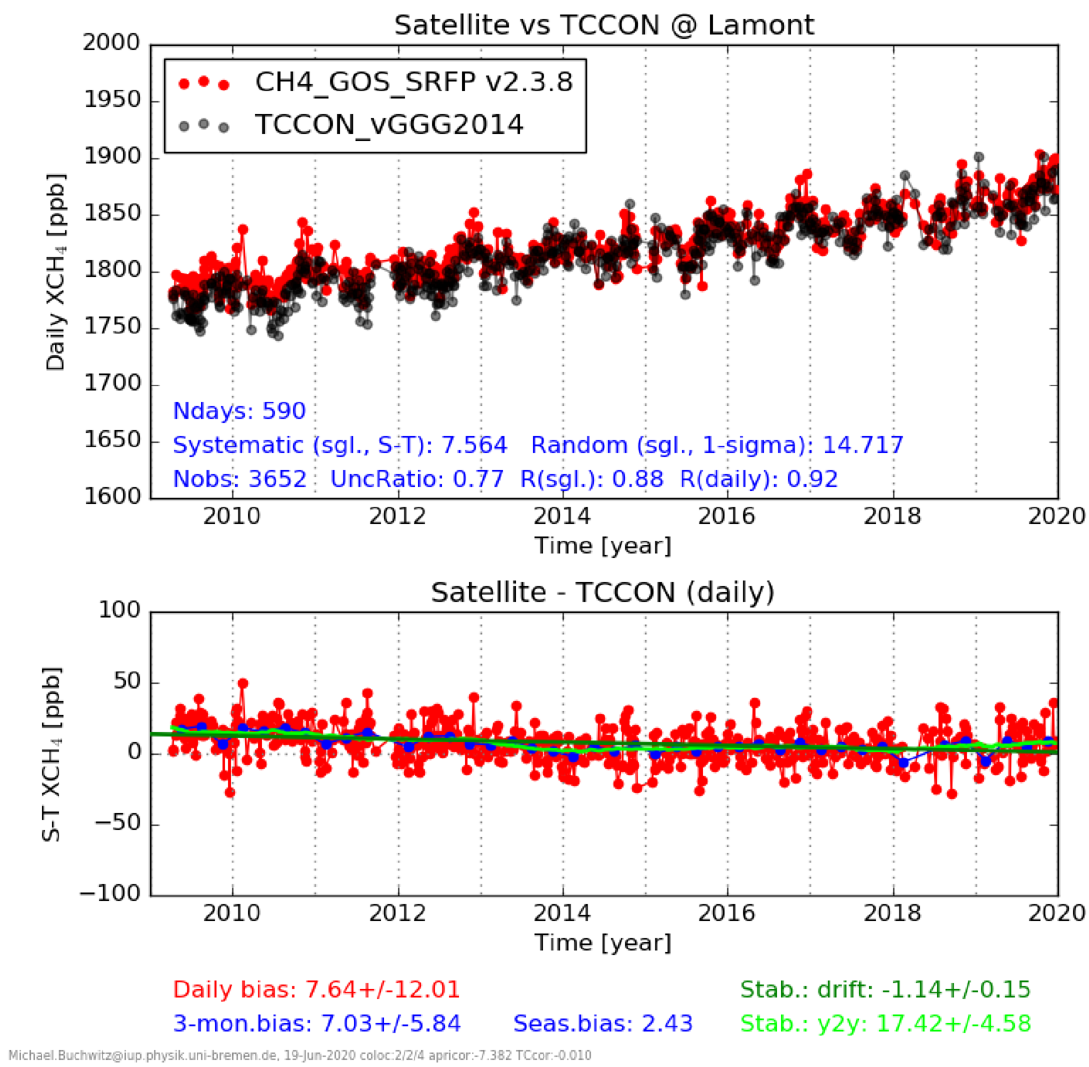


Figure 30 – As **Figure 10** but for product CH4_GOS_SRFP.

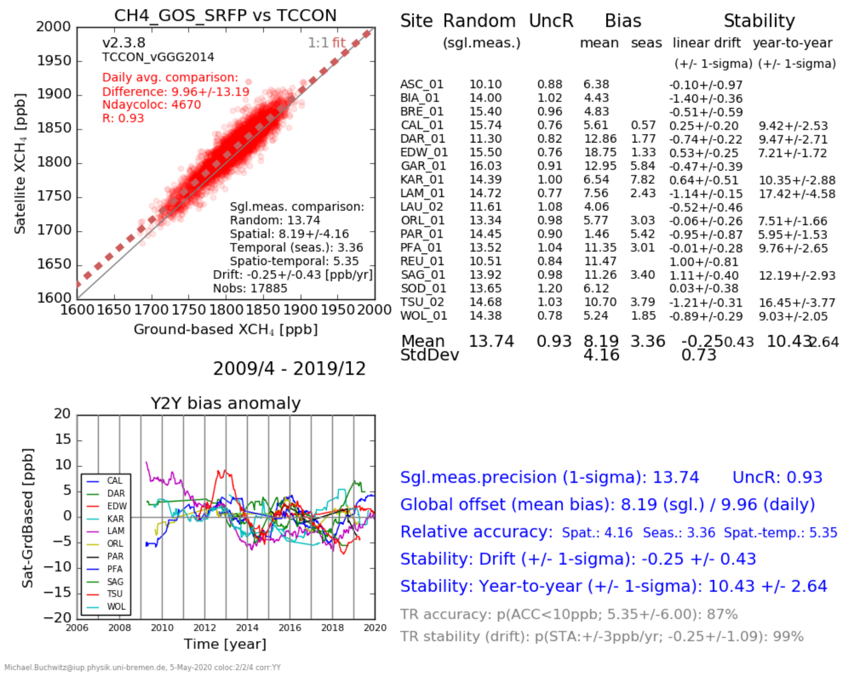


Table 18 - Product Quality Summary Table for product CH4_GOS_SRFP.

Product Quality Summary Table for Product: CH4_GOS_SRFP Level: 2, Version: 2.3.8, Time period covered: 4.2009 – 12.2019				
Parameter [unit]	Achieved performance	Requirement	TR	Comments
Single measurement precision (1-sigma) in [ppb]	14	< 34 (T) < 17 (B) < 9 (G)	-	-
Uncertainty ratio) in [-]: Ratio reported uncertainty to standard deviation of satellite-TCCON difference	0.93	-	-	No requirement but value close to unity expected for a high quality data product.
Mean bias [ppb]	4.2	-	-	No requirement but value close to zero expected for a high quality data product.
Accuracy: Relative systematic error [ppb]	Spatial – spatiotemporal: 4.2 – 5.4	< 10	Probability that accuracy TR is met: 87%	-
Stability: Linear bias trend [ppb/year]	-0.25 +/- 0.43 (1-sigma)	< 3	Probability that stability TR is met: 99%	-
Stability: Year-to-year bias variability [ppb/year]	10 +/- 3 (1-sigma)	< 3	-	-

3.2.7 Validation results for product XCH4_EMMA

Similar figures as shown in 3.1.1 for product CO2_SCI_BESD are shown in this section but for product CH4_GOS_OCFP.

The Product Quality Summary Table for product CH4_GOS_SRFP is shown as Table 18.

Figure 31 - As Figure 9 but for product XCH4_EMMA. The large scatter before mid 2009 is due to the worse performance of SCIAMACHY compared to GOSAT.

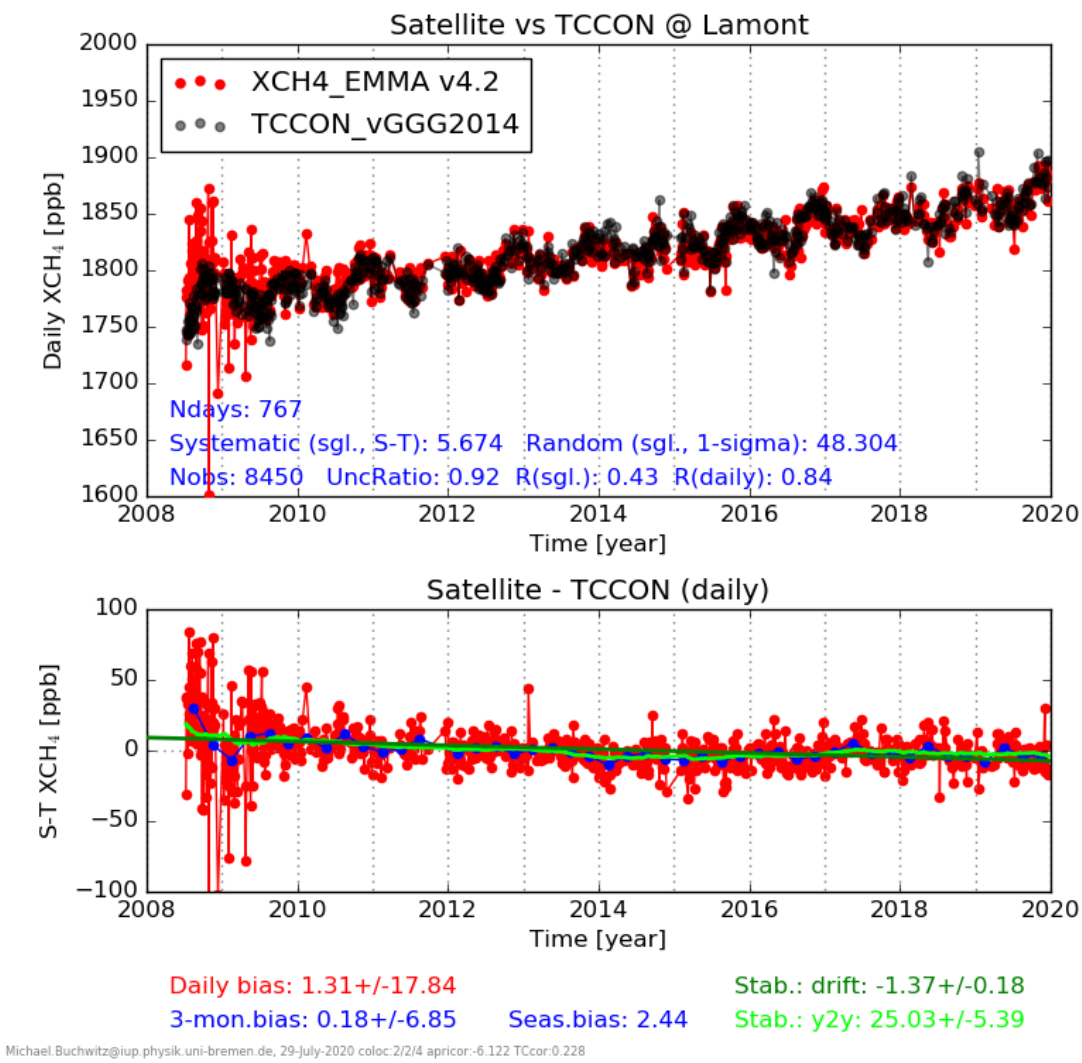


Figure 32 – As **Figure 10** but for product XCH4_EMMA. The “outliers” are due to SCIAMACHY only data before mid 2009.

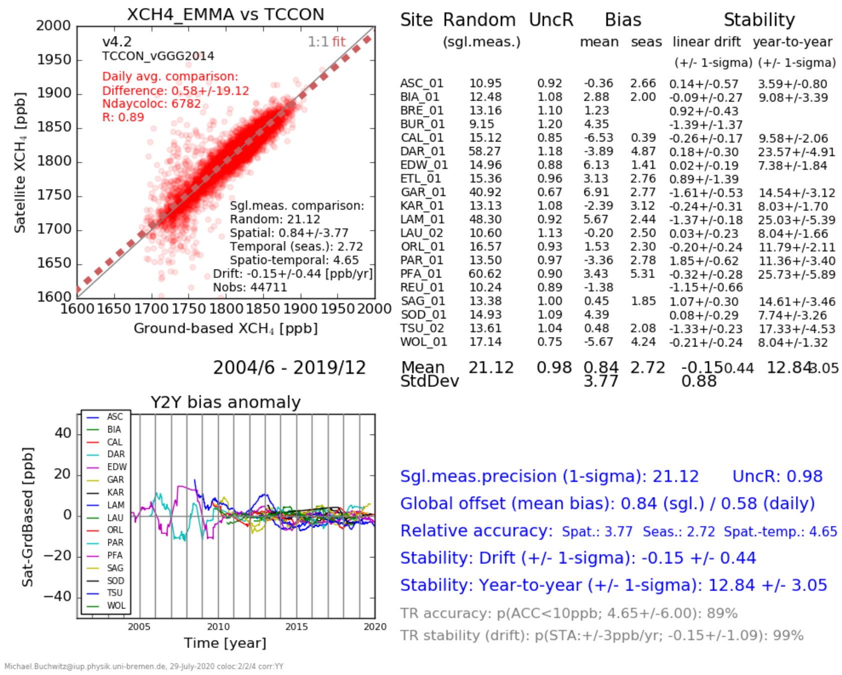


Table 19 - Product Quality Summary Table for product XCH4_EMMA.

Product Quality Summary Table for Product: XCH4_EMMA Level: 2, Version: 4.2, Time period covered: 1.2003 – 12.2019				
Parameter [unit]	Achieved performance	Requirement	TR	Comments
Single measurement precision (1-sigma) in [ppb]	21.1	< 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]	0.84	-	-	No requirement but value close to zero expected for a high quality data product.
Accuracy: Relative systematic error [ppb]	Spatial – spatiotemporal: 3.8 – 4.7	< 10	Probability that accuracy TR is met: 89%	-
Stability: Linear bias trend [ppb/year]	-0.15 +/- 0.44 (1-sigma)	< 3	Probability that stability TR is met: 99%	-
Stability: Year-to-year bias variability [ppb/year]	13 +/- 3 (1-sigma)	< 3	-	-

3.3 Validation results for Level 3 XCO_2 product

In order to validate this product, it has been compared with Total Carbon Column Observation Network (TCCON, *Wunch et al., 2011*) ground-based XCO_2 retrievals using version GGG2014 (*Wunch et al., 2015*).

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 33 shows an overview about all validation results.

Table 20 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 1.2 ppm and the mean bias is -0.11 ppm. Relative systematic errors, i.e., spatial and temporal biases amount to 0.7±0.6 ppm. The computed linear drift of -0.07±0.20 ppm is small and not significant.

Figure 33 – Overview validation results product XCO2_OBS4MIPS.

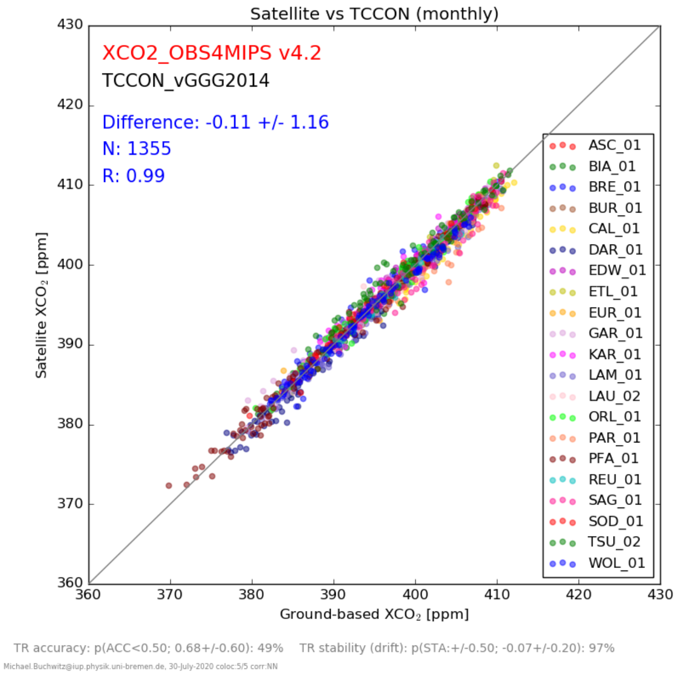


Table 20 – Product Quality Summary Table for product XCO2_OBS4MIPS.

Product Quality Summary Table for Product: XCO2_OBS4MIPS Level: 3, Version: 4.2, Time period covered: 1.2003 – 12.2019				
Parameter [unit]	Achieved performance	Requirement	TR	Comments
Overall uncertainty [ppm]	1.2	-	-	No requirement but small value expected for a high quality data product.
Mean bias [ppm]	-0.11	-	-	No requirement but value close to zero expected for a high quality data product.
Accuracy: Relative systematic error [ppm]	Spatio-temporal bias: 0.7 +/- 0.6 (1-sigma)	< 0.5	Probability that accuracy TR is met: 49%	-
Stability: Linear bias trend [ppm/year]	-0.07 +/- 0.20 (1-sigma)	< 0.5	Probability that stability TR is met: 97%	-

3.4 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 XCO_2 retrievals using version GGG2014 (*Wunch et al., 2015*).

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 34 shows an overview about all validation results.

Table 21 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 8.8 ppb and the mean bias is -3.3 ppb. Relative systematic errors, i.e., spatial and temporal biases amount to 5±6 ppb. The computed linear drift of 0.1±1.0 ppb is small and not significant.

Figure 34 – Overview validation results product XCH4_OBS4MIPS.

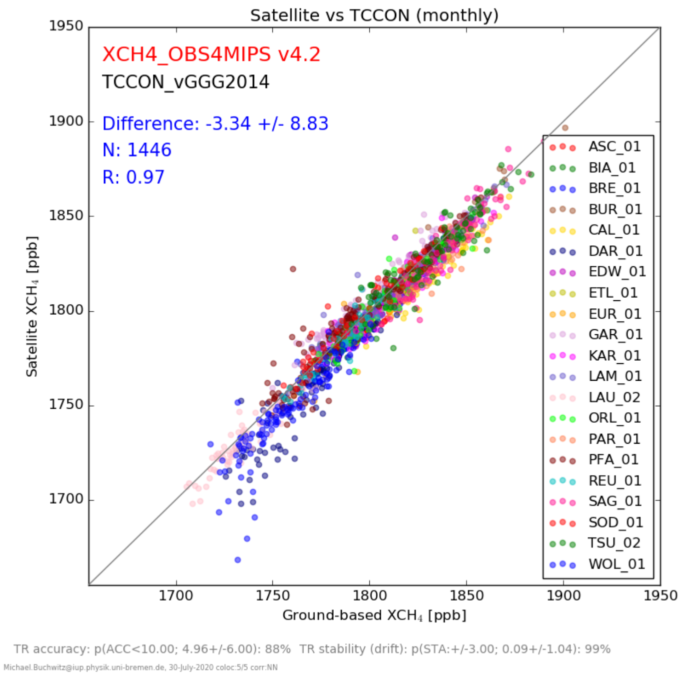


Table 21 – Product Quality Summary Table for product XCH4_OBS4MIPS.

Product Quality Summary Table for Product: XCH4_OBS4MIPS Level: 3, Version: 4.2, Time period covered: 1.2003 – 12.2019				
Parameter [unit]	Achieved performance	Requirement	TR	Comments
Overall uncertainty [ppm]	8.8	-	-	No requirement but small value expected for a high quality data product.
Mean bias [ppb]	-3.3	-	-	No requirement but value close to zero expected for a high quality data product.
Accuracy: Relative systematic error [ppb]	Spatio-temporal bias: 5.0 +/- 6.0 (1-sigma)	< 10	Probability that accuracy TR is met: 88%	-
Stability: Linear bias trend [ppb/year]	0.1 +/- 1.0 (1-sigma)	< 3	Probability that stability TR is met: 99%	-

3.5 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 22 - Table 24.

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 0.57 ppm. The product appears to meet the “relative systematic error” requirement of better than 0.5 ppm: the estimated relative accuracy is in the range 0.46-0.49 ppm. The product is also very stable (-0.01 +/- 0.01 ppm/year (1-sigma)) meeting the requirement for long-term drift. The performance of product CO2_IASB_NLIS (from IASI on Metop-B) seems to be 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 -1.3 ppb. The product appears to meet the “relative systematic error” requirement of better than 10 ppb: the estimated relative accuracy is 5.2 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) seems to be similar.

For product CO2_AIRS_NLIS (from project GHG-CCI) the estimated performance is: single measurement precision: 1.3 ppm, mean bias: -0.43 ppm.

Table 22 - 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 – 12.2019				
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 23 - 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 – 12.2019				
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	-	

Table 24 - Product Quality Summary Table for products CO2_AIRS_NLIS.

Product Quality Summary Table for Product: CO2_AIRS_NLIS Level: 2, Version: 3.0, Time period covered: 4.2003 – 7.2007				
Parameter [unit]	Achieved performance	Requirement	TR	Comments
Single measurement precision (1-sigma) in [ppb]	1.32	< 8 (T) < 3 (B) < 1 (G)	-	-
Mean bias [ppb]	-0.43	-	-	No requirement but value close to zero expected for a high quality data product.

4. Application(s) specific assessments

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

Note however, that the ESA GHG-CCI project pre-cursor data sets have been used for many applications related to the natural and anthropogenic sources and sinks of atmospheric carbon dioxide and methane (e.g., *Reuter et al., 2020*, and references given therein).

The previous C3S data set (CDR1, 2003-2016) has been used for the peer-reviewed publication *Buchwitz et al., 2018*. They analysed the initial C3S XCO_2 Obs4MIPs data product to compute and investigate annual mean XCO_2 growth rates. Their study can be summarized as follows:

“The growth rate of atmospheric carbon dioxide (CO_2) reflects the net effect of emissions and uptake resulting from anthropogenic and natural carbon sources and sinks. Annual mean CO_2 growth rates have been determined globally and for selected latitude bands from satellite retrievals of column-average dry-air mole fractions of CO_2, i.e., XCO_2, for the years 2003 to 2016. The global XCO_2 growth rates agree with National Oceanic and Atmospheric Administration (NOAA) growth rates from CO2 surface observations within the uncertainty of the satellite-derived growth rates (mean difference ± standard deviation: 0.0±0.24ppm/year; R: 0.87). This new and independent data set confirms record large growth rates around 3 ppm/year in 2015 and 2016, which are attributed to the 2015/2016 El Niño. Based on a comparison of the satellite-derived growth rates with human CO_2 emissions from fossil fuel combustion and with El Niño Southern Oscillation (ENSO) indices, we estimate by how much the impact of ENSO dominates the impact of fossil fuel burning related emissions in explaining the variance of the atmospheric CO_2 growth rate.”

Using the XCO2_OBS4MIPS version 4.1 data product the satellite-derived XCO_2 growth rate time series has been updated and extended using the method described in *Buchwitz et al., 2018*. The results are shown in Figure 35. As can be seen from panel (b), the satellite-derived growth rates agree with the NOAA growth rates within the error bar (1-sigma) of the satellite-derived growth rates as also shown for the previous data set (see the detailed discussion in *Buchwitz et al., 2018*). As can be seen, the estimated XCO_2 year 2018 growth rate is 2.1 +/- 0.5 ppm/year (NOAA: 2.43 +/- 0.08 ppm/year). For details see *Reuter et al., 2020*.

The method of *Buchwitz et al., 2018*, has now also been applied to the satellite methane observations using product XCH4_OBS4MIPS version 4.1. The results are shown in Figure 36. As can be seen, the agreement with NOAA is much better for 2010 and later years, i.e., for the time period where GOSAT data have been added. Before 2010 the product is entirely based on SCIAMACHY retrievals, which are less precise and accurate compared to the GOSAT retrievals. Note also that the satellite product is based on an ensemble of several satellite-derived methane products since 2010 and this is expected to also increase the quality of this data product. During the 2010-2018 time period the average XCH_4 increase is 7.9 ±0.2 ppb. For details see Reuter et al., 2019.

Figure 35 – (a) Monthly mean XCO_2 time series 2003-2018., (b) Corresponding annual growth rates (red) compared to NOAA growth rates obtained from surface CO_2 observations (blue; source: https://www.esrl.noaa.gov/gmd/ccgg/trends/gl_gr.html; access: 30-Jul-2019). From: Reuter et al., 2020.

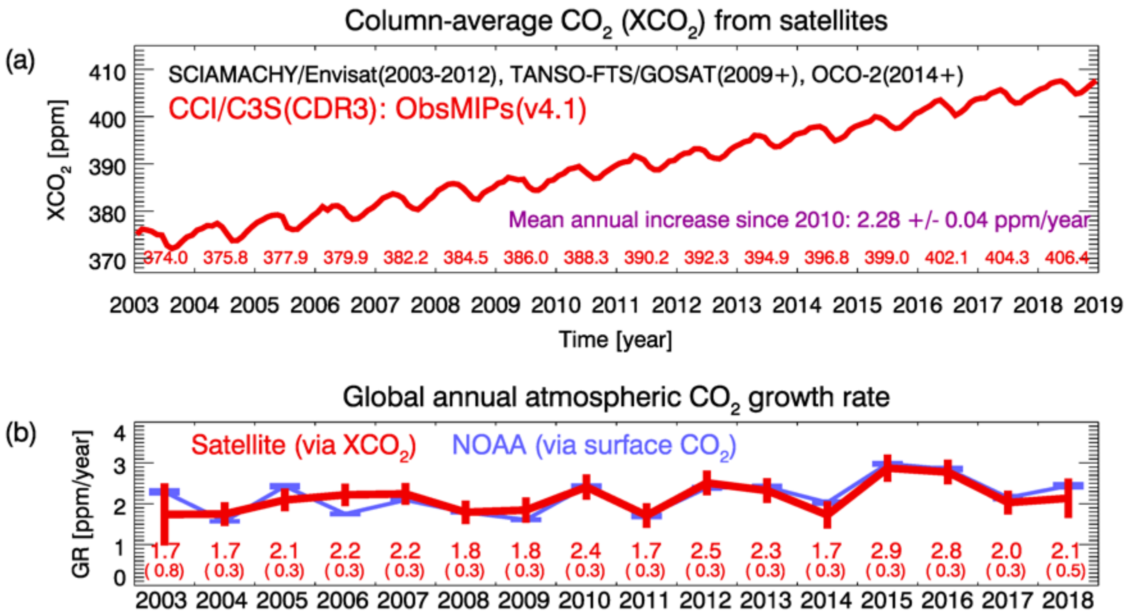
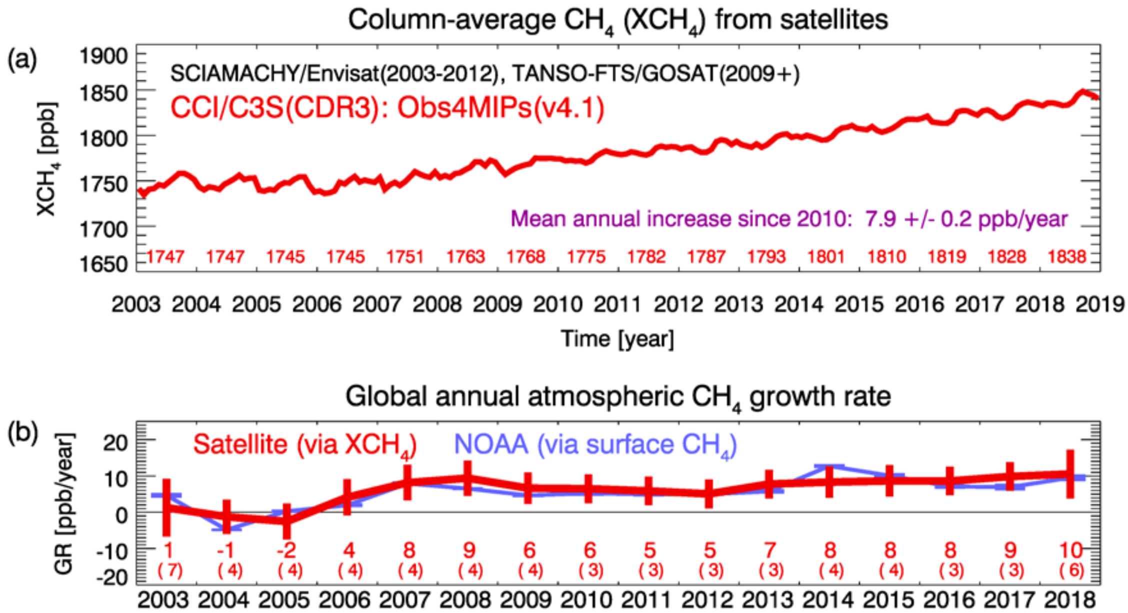


Figure 36 – (a) Monthly mean XCH_4 time series 2003-2018., (b) Corresponding annual growth rates (red) compared to NOAA growth rates obtained from surface CH_4 observations (blue; source: ftp://aftp.cmdl.noaa.gov/products/trends/ch4/ch4_gr_gl.txt; access: 30-Jul-2019). From: Reuter et al., 2020.



5. Compliance with user requirements

5.1 Level 2 XCO_2 and XCH_4 products

XCO_2:

Figure 1 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).

As can be seen, the achieved single observation random error (or precision) is on the order of 1.5 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 between 43% and 69%, depending on product.

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 larger than 86% for all products.

XCH_4:

Figure 2 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).

As can be seen, the achieved single observation random error (or precision) is better than 17 ppb, which is the breakthrough (B) requirement, for the GOSAT and the EMMA products. For SCIAMACHY the precision is worse (50-100 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. For SCIAMACHY the achieved accuracy is around 10 ppb.

Stability is very good for all products. No significant linear bias drift has been detected. The probability that the threshold (T) stability requirement of 3 ppb/year is met is larger than 62% for the SCIAMACHY products and larger than 97% for the other products.

5.2 Level 3 XCO_2 and XCH_4 products

The quality assessment results for the XCO_2 product XCO2_OBS4MIPS are:

The validation of Level 3 product XCO2_OBS4MIPS can be summarized as follows: The overall monthly mean uncertainty is 1.2 ppm and the mean bias is -0.11 ppm. Relative systematic errors, i.e., spatial and temporal biases amount to 0.7±0.6 ppm. The computed linear drift of -0.07±0.20 ppm is small and not significant.

The probability that the 0.5 ppm accuracy requirement is met is 49%.

The probability that the 0.5 ppm/year stability requirement is met is 97%.

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

The quality assessment results for the XCH_4 product XCH4_OBS4MIPS are:

The validation of Level 3 product XCH4_OBS4MIPS can be summarized as follows: The overall monthly mean uncertainty is 8.8 ppb and the mean bias is -3.3 ppb. Relative systematic errors, i.e., spatial and temporal biases amount to 5±6 ppb. The computed linear drift of 0.1±1.0 ppb is small and not significant.

The probability that the 10 ppb accuracy requirement is met is 88%.

The probability that the 3 ppb/year stability requirement is met is 99%.

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

5.3 Level 2 mid-tropospheric products

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) seems to be 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) seems to be similar.

For product CO2_AIRS_NLIS (from project GHG-CCI) the estimated performance is: single measurement precision: 1.3 ppm, mean bias: -0.43 ppm.

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7. List of ANNEXes

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

7.1 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.

7.2 ANNEX B: PQAR for products CO2_GOS_SRFP, CH4_GOS_SRFP

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

7.3 ANNEX C: PQAR for product CH4_GOS_SRPR

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

7.4 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.

7.5 ANNEX E: PQAR for IASI CO_2 and CH_4 and AIRS CO_2 products

Describes the validation of the mid-tropospheric CO_2 and CH_4 products from the IASI instrument series and AIRS 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/

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