ECMWF COPERNICUS REPORT

Copernicus Climate Change Service

Product Quality Assessment Report (PQAR) – Main document

C3S_312a_Lot6_IUP-UB – Greenhouse Gases

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Institute of Environmental Physics (IUP)

Date: 20/10/2017

Ref: C3S_D312a_Lot6.3.1.7-v1_PQAR_v1.1

Official reference number service contract: 2016/C3S_312a_Lot6_IUP-UB/SC1

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History of modifications

Version	Date	Description of modification	Chapters / Sections
1.0	29-September-2017	New document	All
1.0b	11-October-2017	Page header logo replaced	Page header
1.1	20-October-2017	KPI replaced by TR Update of TRD reference	All

Related documents

Reference ID	Document
D1	**GCOS-154:** Global Climate Observing System (GCOS), SYSTEMATIC OBSERVATION REQUIREMENTS FOR SATELLITE-BASED PRODUCTS FOR CLIMATE, 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)", Prepared by World Meteorological Organization (WMO), Intergovernmental Oceanographic Commission, United Nations Environment Programme (UNEP), International Council for Science, Doc.: GCOS 154, link: https://www.wmo.int/pages/prog/gcos/Publications/gcos-154.pdf, 2010.
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, link: http://www.esa-ghg-cci.org/?q=webfm_send/344, 2016.
D4	**TRD GHG, 2017:** Buchwitz, M., Aben, I., Anand, J., Armante, R., Boesch, H., Crevoisier, C., Detmers, R. G., Hasekamp, O. P., Reuter, M., Schneising-Weigel, O., Target Requirement 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_312a_Lot6), Version 1.3, 20-October-2017, pp. 53, 2017.
D5	**ATBD GHG, 2017:** Buchwitz, M., Aben, I., Anand, J., Armante, R., Boesch, H., Crevoisier, C., Detmers, R. G., Hasekamp, O. P., Reuter, M., Schneising-Weigel, O., Algorithm Theoretical Basis Document (ATBD) – Main document, C3S project C3S_312a_Lot6_IUP-UB – Greenhouse Gases, 2017.
D6	**PUGS GHG, 2017:** Buchwitz, M., Aben, I., Anand, J., Armante, R., Boesch, H., Crevoisier, C., Detmers, R. G., Hasekamp, O. P., Reuter, M., Schneising-Weigel, O., Product User Guide and Specification (PUGS) – Main document, C3S project C3S_312a_Lot6_IUP-UB – Greenhouse Gases, 2017.

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
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 GHG, 2017*, *ESA-CCI-GHG-URDv2.1* and *CMUG-RBD, 2010*:

<u>Systematic error</u>: 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:

<u>Relative systematic error</u>: Identical with “Systematic error” but after bias correction.

<u>Bias</u>: estimate of a systematic measurement error (*JCGM, 2008*).

<u>Precision</u> 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 GHG, 2017*) 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 project C3S_312a_Lot6 led by University of Bremen, Germany.

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).

Requirements on data quality are formulated in the corresponding Target Requirement Document (TRD) (*TRD GHG, 2017*).

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.

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_312a_Lot6 project of the Copernicus Climate Change Service (C3S, https://climate.copernicus.eu/) is described.

The C3S_312a_Lot6 satellite-derived 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). 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 GHG, 2017*).

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 GHG, 2017*) 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 (http://www.esa-ghg-cci.org/) of ESA's Climate Change Initiative (CCI). The main goal of the C3S_312a_Lot6 project is to extend (in time) the data base of GHG-CCI pre-cursor data products. The first C3S_312a_Lot6 data set, described in this document, covers the time period 2003-2016. This data set and its documentation is available via the C3S CDS.

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 (University of Bremen's merged Level 2 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 2 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.

Table 2 - 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	32%	90%	3.1.1
CO2_SCI_WFMD	2	XCO_2 from SCIAMACHY retrieved using Univ. Bremen's WFMD algorithm	9%	96%	3.1.2
CO2_GOS_OCFP	2	XCO_2 from GOSAT retrieved using Univ. Leicester's OCFP algorithm	29%	96%	3.1.3
CO2_GOS_SRFP	2	XCO_2 from GOSAT retrieved using SRON's SRFP (RemoTeC) algorithm	30%	98%	3.1.4
XCO2_EMMA	2	Merged multi-satellite XCO_2 via Univ. Bremen's EMMA algorithm	37%	98%	3.1.7
XCO2_OBS4MIPS	3	Merged multi-satellite XCO_2 via Univ. Bremen's OBS4MIPS algorithm	76%	99%	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	43%	62%	3.2.1
CH4_SCI_IMAP	2	XCH_4 from SCIAMACHY retrieved using the IMAP algorithm of SRON/JPL	55%	98%	3.2.2
CH4_GOS_OCPR	2	XCH_4 from GOSAT retrieved using Univ. Leicester's OCPR	100%	96%	3.2.3

		algorithm			
CH4_GOS_SRPR	2	XCH_4 from GOSAT retrieved using SRON's SRPR (RemoTeC) algorithm	100%	98%	3.2.4
CH4_GOS_OCFP	2	XCH_4 from GOSAT retrieved using Univ. Leicester's OCFP algorithm	97%	94%	3.2.5
CH4_GOS_SRFP	2	XCH_4 from GOSAT retrieved using SRON's SRFP (RemoTeC) algorithm	100%	98%	3.2.6
XCH4_EMMA	2	Merged multi-satellite XCH_4 via Univ. Bremen's EMMA algorithm	96%	95%	3.2.7
XCH4_OBS4MIPS	3	Merged multi-satellite XCH_4 via Univ. Bremen's OBS4MIPS algorithm	100%	97%	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	100%	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	100%	-	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.

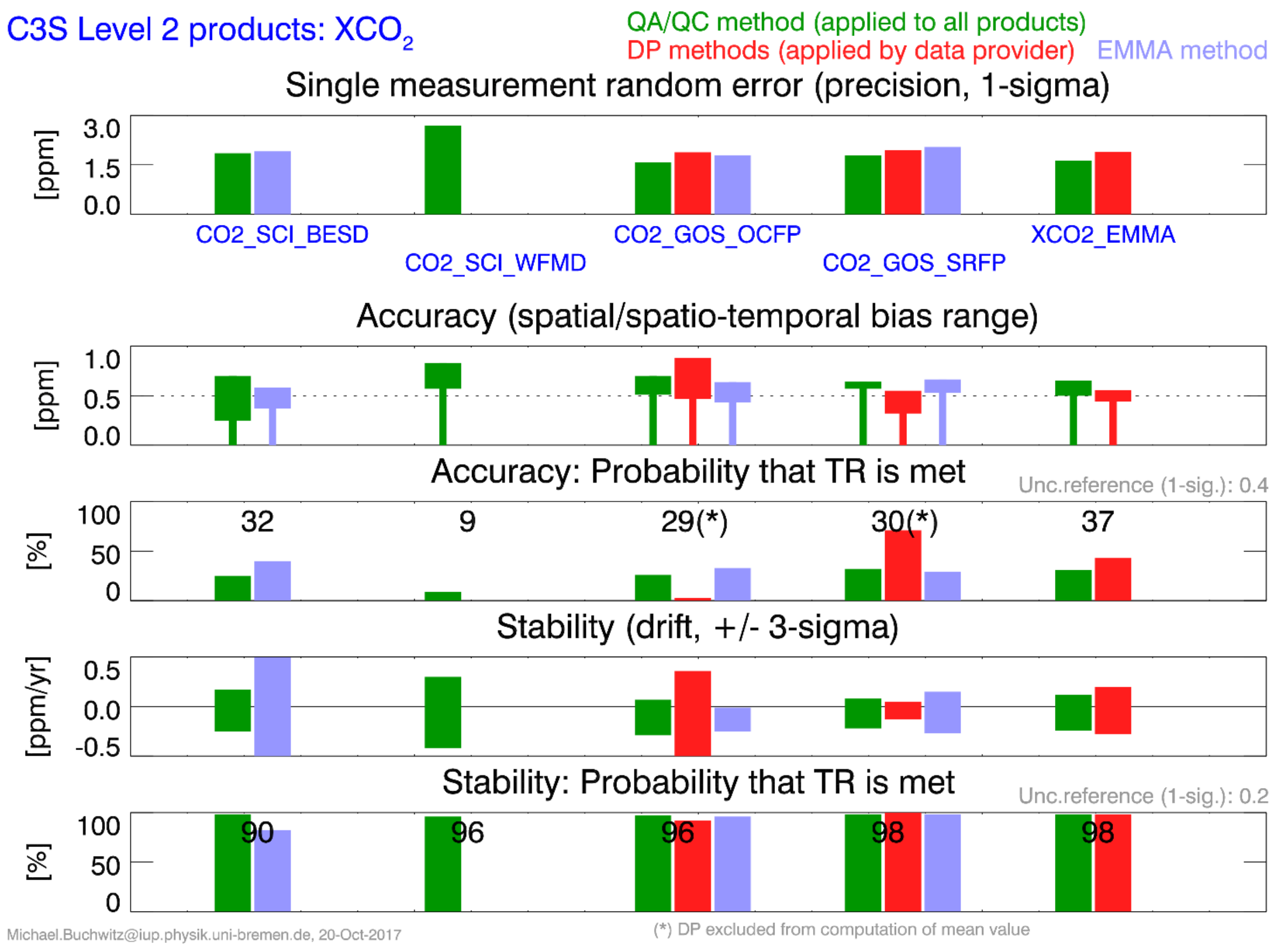
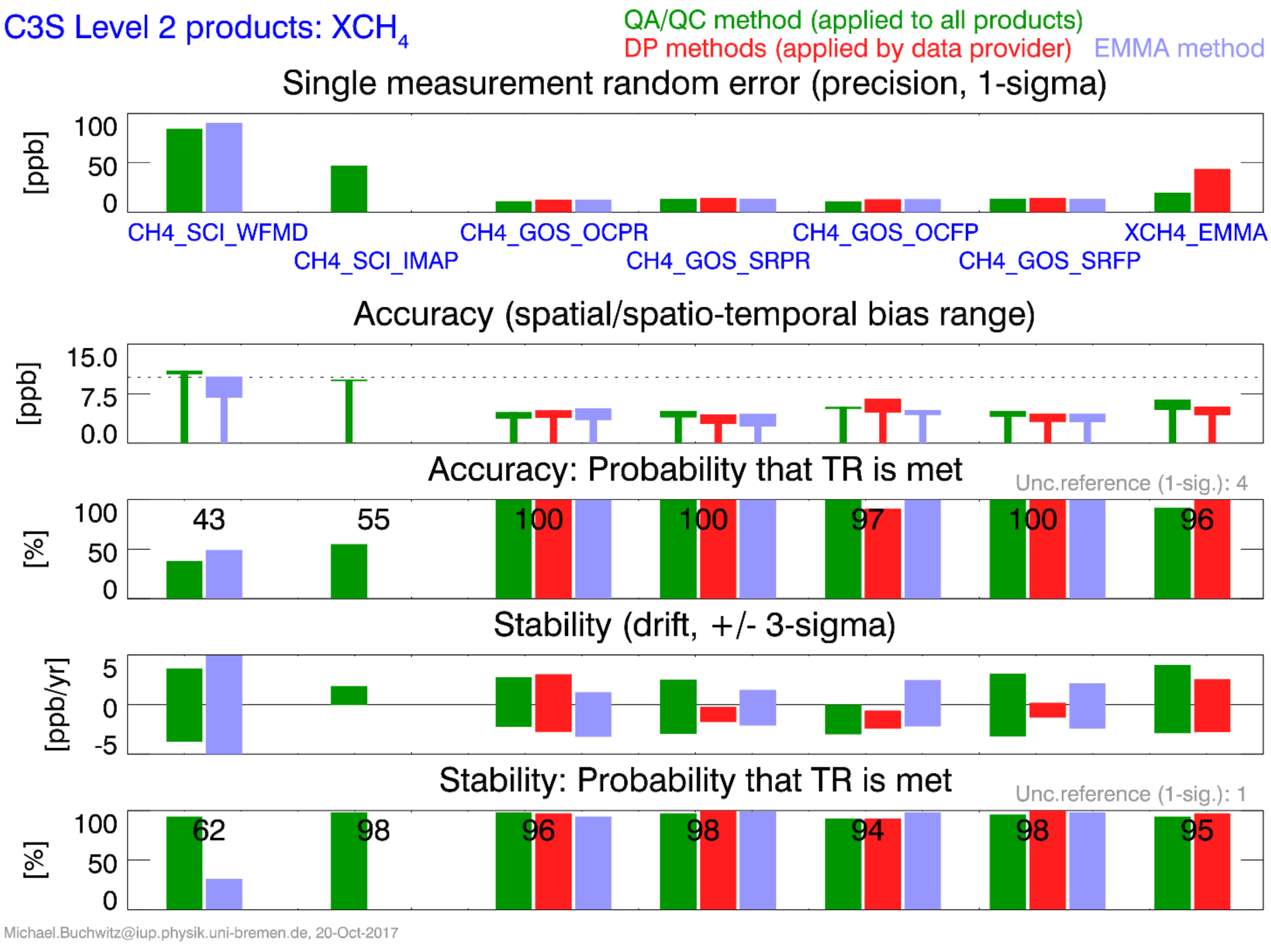


Figure 2 - Overview data quality assessment results for Level 2 XCH_2 data products. The green bars refer to the "Quality Assessment / Quality control" (QA/QC) results as described in this document. The red bars refer to results obtained by the data providers (DPs), as described in separate Annexes (see 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.



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*):

- 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.

Currently data from two of these instruments – SCIAMACHY and TANSO-FTS - have been used to generate the Level 2 XCO_2 and XCH_4 data products described and assessed in this document. Data products from additional sensors may be added in the future.

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/.

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. At the time of writing only limited information on the achieved in-orbit XCO_2 performance of TanSat is available.

1.1.2.5 Sentinel-5-Precursor (S5P)

ESA's Sentinel-5-Precursor (S5P) mission (*Veefkind et al, 2012*) is scheduled for launch in mid 2017. S5P will permit XCH_4 retrievals (*Butz et al., 2012*) 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.

1.1.2.6 Other instruments

Several other satellites are expected to be launched in the future, e.g., the GOSAT follow-on GOSAT-2 for XCO_2 and XCH_4, the active laser-based mission MERLIN (Methane Remote Sensing Lidar Mission, see https://de.wikipedia.org/wiki/Merlin_(Satellit)) for XCH_4 and NASA's recently approved geostationary GeoCARB mission. It can also be expected that in the future other satellites will be launched which permit also to obtain detailed global information on anthropogenic CO_2 emissions (e.g., *Ciais et al., 2015*), for example a satellite like CarbonSat (*Bovenmann et al., 2010; Buchwitz et al., 2013b; Pillai et al., 2016*) or even a CarbonSat-like constellation (*Velazco et al., 2011*).

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., 201*3). 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, **Fehler! Verweisquelle konnte nicht gefunden werden.** 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 4 shows maps and time series for two of these products.

Figure 3 – Satellite-derived northern hemispheric 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.

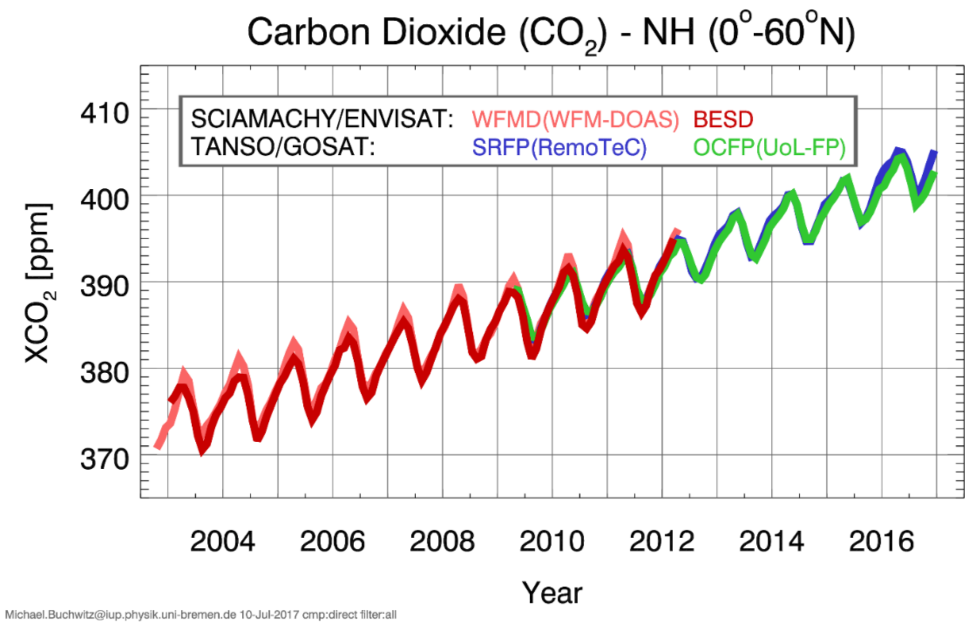
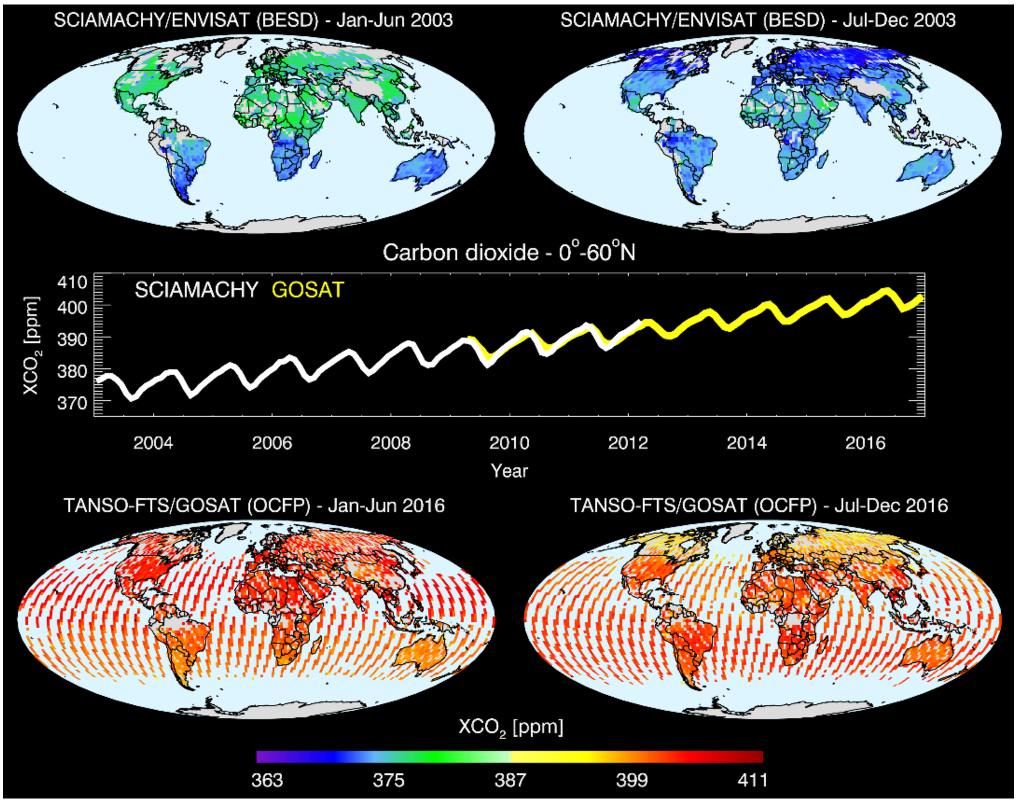


Figure 4 - Maps of XCO_2 product CO2_SCI_BESD (top, for year 2003) and product CO2_GOS_OCFP (bottom, for year 2016) and northern hemispheric time series (middle).



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 5 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 6 shows maps and time series for two of these products.

Figure 5 – Satellite-derived northern hemispheric 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.

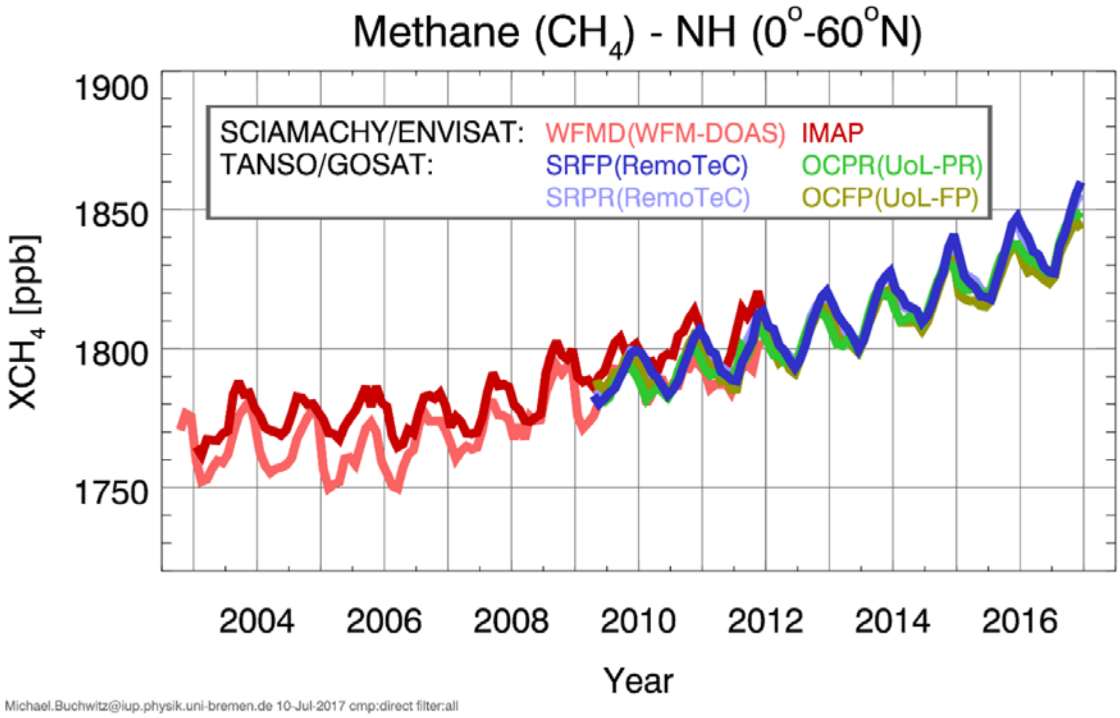
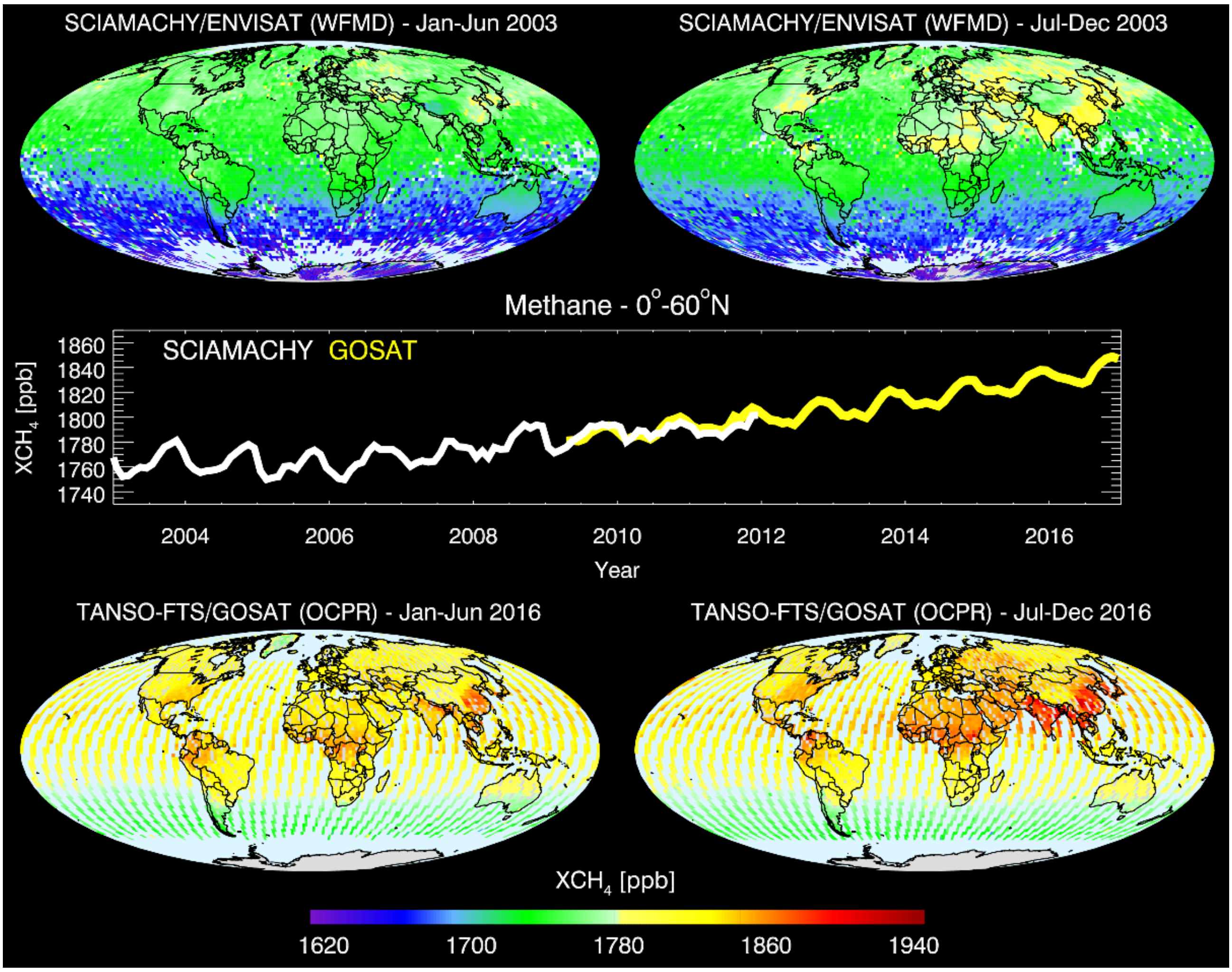


Figure 6 - Maps of XCH_4 product CH4_SCI_WFMD (top, 2003) and product CH4_GOS_OCPR (bottom, 2016) and northern hemispheric time series (middle).



1.1.5 List of XCO_2 and XCH_4 data products

Table 3 and Table 4 list the XCO_2 and XCH_4 data products, respectively.

As can be seen from Table 3, 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 GHG-CCI project (http://www.esa-ghg-cci.org/). They are available via the C3S CDS but are also available from the GHG-CCI website (http://www.esa-ghg-cci.org/) including documentation. They are used within project C3S_312a_Lot6 to generate the merged Level 2 ("EMMA") and Level 3 ("OBS4MIPs") products.

Table 3 - 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	
CO2_GOS_SRFP	2	GOSAT	Oct. 2017: 2009-2016 Oct. 2018: 2009-2017	
CO2_SCI_BESD	2	SCIAMACHY	Feb. 2017: 2003-2011	Existing GHG-CCI product
CO2_SCI_WFMD	2	SCIAMACHY	Feb. 2017: 2003-2011	Existing GHG-CCI product
XCO2_EMMA	2	Merged SCIAMACHY & GOSAT	Oct. 2017: 2003-2016 Oct. 2018: 2003-2017	
XCO2_OBS4MIPS	3	Merged SCIAMACHY & GOSAT	Oct. 2017: 2003-2016 Oct. 2018: 2003-2017	

As can be seen from Table 4, 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 4 - 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	
CH4_GOS_SRPR	2	GOSAT	Oct. 2017: 2009-2016 Oct. 2018: 2009-2017	
CH4_GOS_OCFP	2	GOSAT	Oct. 2017: 2009-2016 Oct. 2018: 2009-2017	
CH4_GOS_SRFP	2	GOSAT	Oct. 2017: 2009-2016 Oct. 2018: 2009-2017	
CH4_SCI_WFMD	2	SCIAMACHY	Feb. 2017: 2003-2011	Existing GHG-CCI product
CH4_SCI_IMAP	2	SCIAMACHY	Feb. 2017: 2003-2011	Existing GHG-CCI product
XCH4_EMMA	2	Merged SCIAMACHY & GOSAT	Oct. 2017: 2003-2016 Oct. 201 : 2003-2017	
XCH4_OBS4MIPS	3	Merged SCIAMACHY & GOSAT	Oct. 2017: 2003-2016 Oct. 2018: 2003-2017	

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 in October 2018. 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 5 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 GHG-CCI project (http://www.esa-ghg-cci.org/). This product exists and is available from the GHG-CCI website (http://www.esa-ghg-cci.org/ -> CRDP (Data)). It will be delivered to ECMWF essentially « as is » (incl. existing documentation) and made available for the C3S CDS. However, it currently only exists in ASCII format but it will be converted to NetCDF format for C3S as will also be done for the IASI products listed in Table 5.

Table 5 - 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 Oct. 2018: 2007-2017	
CH4_IASA_NLIS	2	IASI / Metop-A	Oct. 2017: 2007-2015 Oct. 2018: 2007-2017	
CO2_IASB_NLIS	2	IASI / Metop-B	Oct. 2017: 2013-2016 Oct. 2018: 2013-2017	
CH4_IASB_NLIS	2	IASI / Metop-B	Oct. 2017: 2013-2016 Oct. 2018: 2013-2017	
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 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 (http://www.esa-ghg-cci.org/) of ESA's Climate Change Initiative is called "Climate Research Data Package No. 4" (CRDP4) and is available from the main data products website of the GHG-CCI website (http://www.esa-ghg-cci.org/ -> CRDP (Data) or directly via http://www.esa-ghg-cci.org/sites/default/files/documents/public/documents/GHG-CCI_DATA.html). 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: Computed as the mean difference of the satellite measurements with TCCON.

- "Relative systematic error" (or "relative accuracy"): Computed as standard deviation of the biases as obtained at the various TCCON sites (computed for the entire time series of in additions seasonally resolved).
- 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.
- QA/QC of the reported uncertainties: 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) associated with that observations. To assess the quality of these uncertainty estimates they have been compared with the standard deviation of the satellite minus TCCON retrievals at the various TCCON sites. The ratio of the mean value of the reported uncertainty would be identical with the standard deviation of the difference to TCCON if the reported uncertainty is correct and if the comparison method does not introduce an additional error (which is typically not the case, e.g., due to imperfect co-location in time and space). Therefore, one expects that the ratio of the mean value of the reported uncertainty and the standard deviation of the satellite minus TCCON difference is close (i.e., within a few 10%) to unity and this been typically confirmed for all products.

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 differences (in particular those related to Target Requirements (TR) assessments, which have not been carried out for the pre-cursor products), which are described in the following.

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>QA/QC of the 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.

<u>"Relative systematic error" (or "relative accuracy" or "relative bias" or simply "accuracy"):</u>
Computed as standard deviation of the biases as obtained at the various TCCON sites.
Typically two values are computed and reported (e.g., to be consistent with past assessments):

- Standard deviation of the biases at the selected TCCON sites ("relative spatial bias")
- Standard deviation of the biases at the selected TCCON sites based on time / quarterly resolved (JFM, AMJ, JAS, OND) biases ("relative spatio-temporal bias")

<u>Stability: Linear bias trend (Long term drift):</u>
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. See also document PVIRv5 (*Buchwitz et al., 2017*) for an assessment of this quantity using the pre-cursor products.

<u>Stability: Year-to-year bias variability:</u>
Computed as maximum minus minimum bias difference of smoothed (using a one year running average) satellite minus TCCON differences. See also document PVIRv5 (*Buchwitz et al., 2017*) for an assessment of this quantity using the pre-cursor products.

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 (as also done in the past for the pre-cursor products, see PVIRv5 (*Buchwitz et al., 2017*)):

- 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) (*TRD GHG, 2017*).

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 GHG, 2017*)):

- (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

Accuracy:

As explained earlier, the term "accuracy" as used here means "relative accuracy" or "relative bias" (because a possible "global offset" is not critical for the main application of the data products (namely 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"); note that also a "global offset" (a single constant value per product) has been determined and is reported in this document and can be taken into account by the users if needed).

"Accuracy" is estimated as standard deviation of the biases at the used TCCON validation sites. The estimated value is therefore 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). It is also assumed for the following that the uncertainty of the obtained accuracy value is not known.

The uncertainty of the TCCON reference data is (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*):

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

These values are the assumed minimum uncertainties (“UNC_ACC”) of the estimated accuracy value (“ACC”), i.e., we have ACC +/- UNC_ACC (1-sigma) for the estimated accuracy and its uncertainty.

Note that the uncertainty estimate UNC_ACC can be refined by considering also other uncertainties (e.g., errors due to imperfect co-location etc.). In this case, the overall uncertainty shall be computed as “Root-Sum-Square” (RSS), i.e., the individual uncertainties shall be added quadratically (assuming uncorrelated errors).

ACC is a non-negative number (as it is computed as a standard deviation) and the Target Requirement (TR) for accuracy defines an “acceptable range” or interval of accuracy values: [0, TR[, i.e., in order to meet the requirements ACC shall be smaller than TR (but will be larger or equal zero). Because of this “non-negativity”, ACC cannot be distributed according to a Gaussian probability density function. The probability function PROB(ACC) cannot be defined / pre-scribed in this document (it needs to be obtained empirically) and in practise may be very difficult to obtain. Arguably the simplest but still reasonable assumption is to use a simple box-car function of width two times UNC_ACC (here: two time the 1-sigma TCCON uncertainty listed above).

In order to compute the probability that the accuracy TR is met, P(ACC), the area under the PROB(ACC) function over the [0, TR[interval of required accuracy values needs to be computed. For the box-car assumption (and ignoring negative values) this gives the following function P(ACC):

if ACC > TR + UNC_ACC:	P = 0
if ACC < TR - UNC_ACC:	P = 1
otherwise:	P = 0.5 + 0.5 x (TR – ACC) / UNC_ACC

This is illustrated in Figure 7 for XCO_2 and Figure 8 for XCH_4.

Figure 7 - Probability that the XCO_2 accuracy TR is met as a function of "estimated accuracy" ACC (in ppm) (using ACC_UNC=0.4 ppm).

ACC:	P(TR=met):
0,00	1,00
0,10	1,00
0,20	0,88
0,30	0,75
0,40	0,63
0,50	0,50
0,60	0,38
0,70	0,25
0,80	0,13
0,90	0,00
1,00	0,00

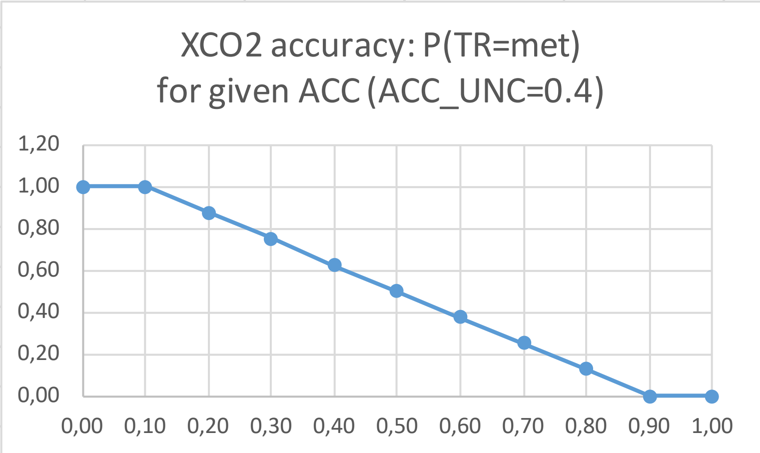
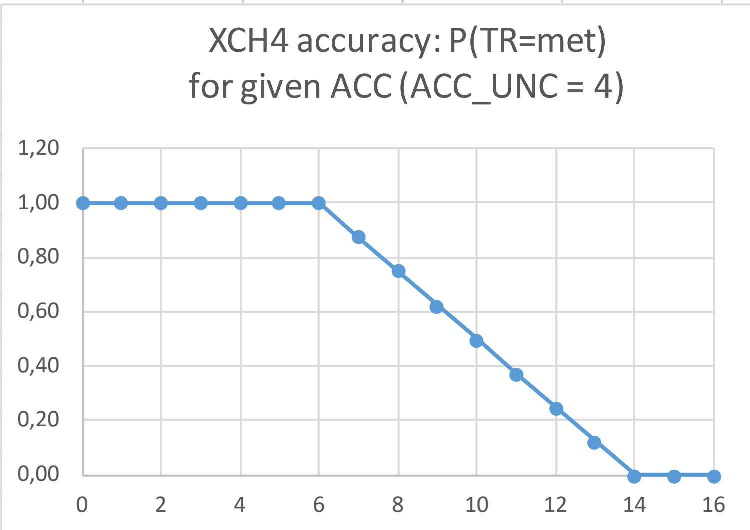


Figure 8 - Probability that the XCH_4 accuracy TR is met as a function of "estimated accuracy" ACC (in ppb) (using ACC_UNC=4 ppb).

ACC:	P(TR=met):
0	1,00
1	1,00
2	1,00
3	1,00
4	1,00
5	1,00
6	1,00
7	0,88
8	0,75
9	0,63
10	0,50
11	0,38
12	0,25
13	0,13
14	0,00
15	0,00
16	0,00



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 one may assume 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), which is shown in Figure 9 for Nc(x, mean=0, sigma=1).

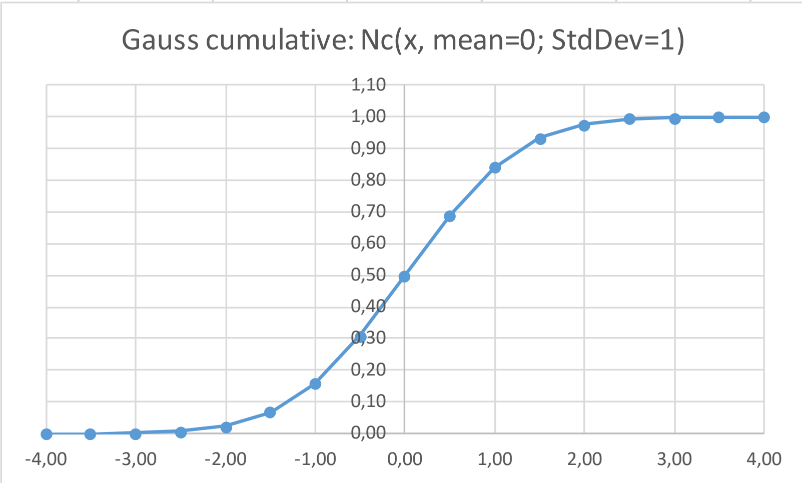
The probability P that the stability TR is met for XCO_2 for a given value of STA is therefore for this example:
P(STA) = Nc(+0.5, mean=+0.1, sigma=0.2) – Nc(-0.5, mean=+0.1, sigma=0.2) = 97%

The probability P that the stability TR is met for XCH_4 for a given value of STA is therefore for this example:
P(STA) = Nc(+3, mean=-0.8, sigma=1.08) – Nc(-3, mean=-0.8, sigma=1.08) = 98%

This means that in these cases it is almost certain that the stability TR is met.

Figure 9 - Cumulative distribution function of a Gaussian probability density function with a mean value of 0.0 and a standard deviation of 1.0.

x	Nc(x,0,1)
-4,00	0,00
-3,50	0,00
-3,00	0,00
-2,50	0,01
-2,00	0,02
-1,50	0,07
-1,00	0,16
-0,50	0,31
0,00	0,50
0,50	0,69
1,00	0,84
1,50	0,93
2,00	0,98
2,50	0,99
3,00	1,00
3,50	1,00
4,00	1,00

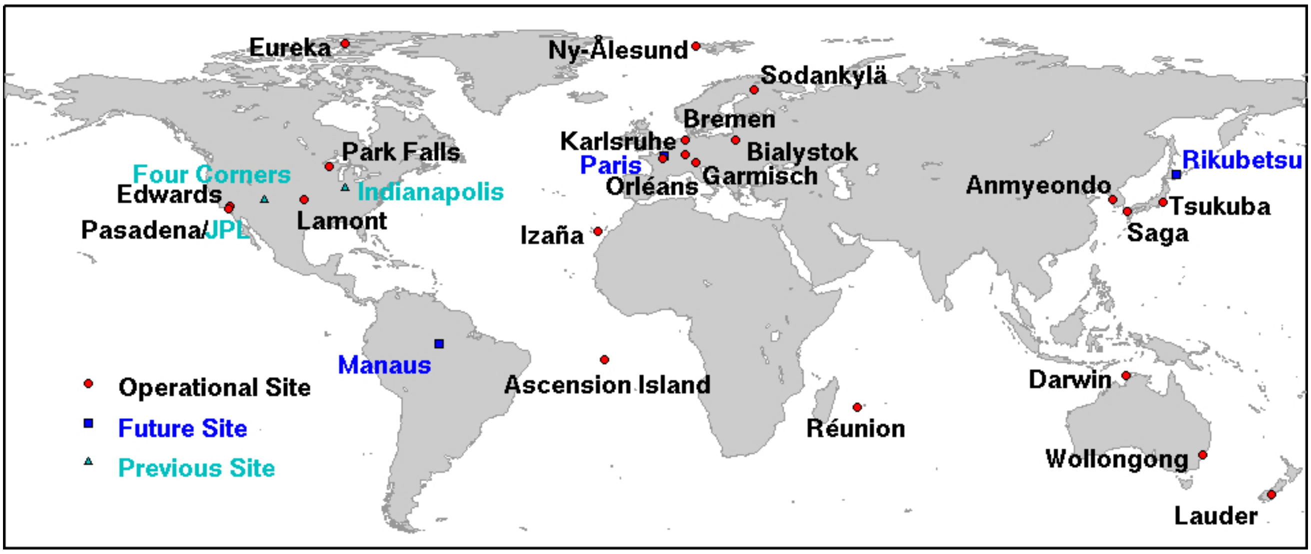


2.2.1.4 Known limitations

2.2.1.4.1 TCCON

The TCCON network consists of about 20 TCCON sites (see Figure 10). 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 10 - Location of TCCON sites. Source: www.cger.nies.go.jp/cgernews/201503/292004.html.



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 (http://www.esa-ghg-cci.org/) 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 GHG, 2017*) 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 (http://www.esa-ghg-cci.org/) of ESA's Climate Change Initiative is called "Climate Research Data Package No. 4" (CRDP4) and is available from the main data products website of the GHG-CCI website (http://www.esa-ghg-cci.org/ -> CRDP (Data) or directly via http://www.esa-ghg-cci.org/sites/default/files/documents/public/documents/GHG-CCI_DATA.html). 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 16 TCCON data set: Ascension, Bialystok, Bremen, Darwin, Garmisch, Izana, Karlsruhe, Lamont, Lauder 1 and 2, Paris, Park Falls, Reunion, Saga, Sodankyla, and Wollongong. Detailed information on each site can be found at https://tccon-wiki.caltech.edu/Sites. The used TCCON version is GGG2014 (data access: 22-June-2017).

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 11 shows the comparison at the TCCON site Lamont (“LAM”), Oklahoma, USA. Please see the figure caption for a detailed explanation of the FoMs resulting from this comparison.

As can be seen from Figure 11 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 a sufficient number of co-locations per season (at least 10 days) and per year (at least 20 days) and overall (at least 60 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 12 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 11). Listed are

- the TCCON site ID (e.g., LAM for Lamont),
- the 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 and seasonal bias (see Figure 11) and
- FoMs characterising stability in terms of drift and year-to-year bias variability (see caption Figure 11 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”, (ii) the standard deviation (“StdDev”) or (iii) as “(max-min)/4”. The latter quantity is used to estimate the 1-sigma uncertainty of the linear drift (assuming that max-min is a good estimate of the 4-sigma uncertainty).

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 12:

- Single measurement precision (1-sigma)
- Uncertainty ratio (“UncR”)
- Accuracy computed as standard deviation of the site-to-site biases as a measure of “regional bias” and also as seasonal bias (to characterize the temporal component of the bias)
- 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 6, which summarizes the quality assessment results for this product.

Figure 11 - 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. Listed are the following figures of merit: mean bias (= mean difference), single measurement precision (standard deviation of the difference of the individual satellite observations and TCCON), 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, the number of satellite observations (“Nobs”) as used for the comparison, the number of days (“Ndays”) used for comparison and the linear correlation coefficient of the daily averaged data (“R(daily)”). Bottom: Daily differences satellite minus TCCON (red symbols). The thick blue line shows the “seasonal bias time series”, which is the 3 months mean bias (running average). The standard deviation of the values of this curve is the seasonal bias (“Seas.bias”). The light blue line is a linear fit and the slope and its (1-sigma) uncertainty are listed as “Stab.: drift” characterizing the linear drift of the bias (in ppm/year). A second measure of stability is the year-to-year bias variability, which is the maximum minus minimum value of the green curve, which shows the yearly mean bias (running average). The numerical results are listed as “Stab.: y2y” (also in ppm/year) in terms of value and its uncertainty (computed from the standard deviation of the daily biases in one year time periods).

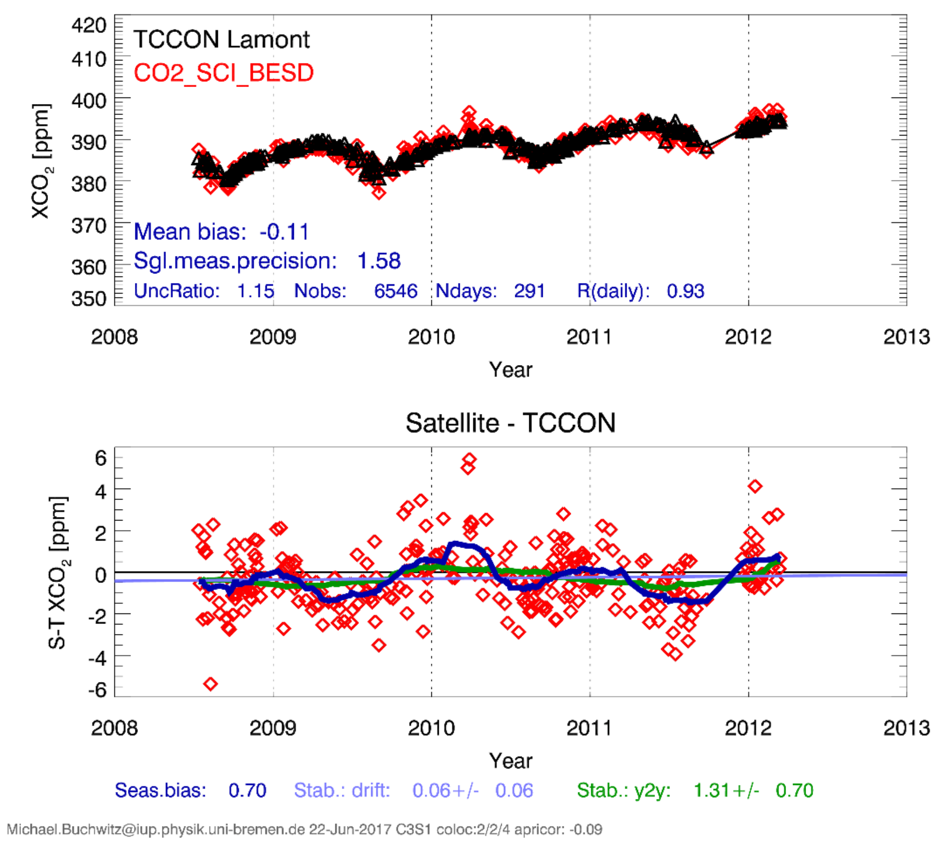


Figure 12 - Product Quality Summary Figure for product CO2_SCI_BESD. Please see the main text for a detailed explanation.

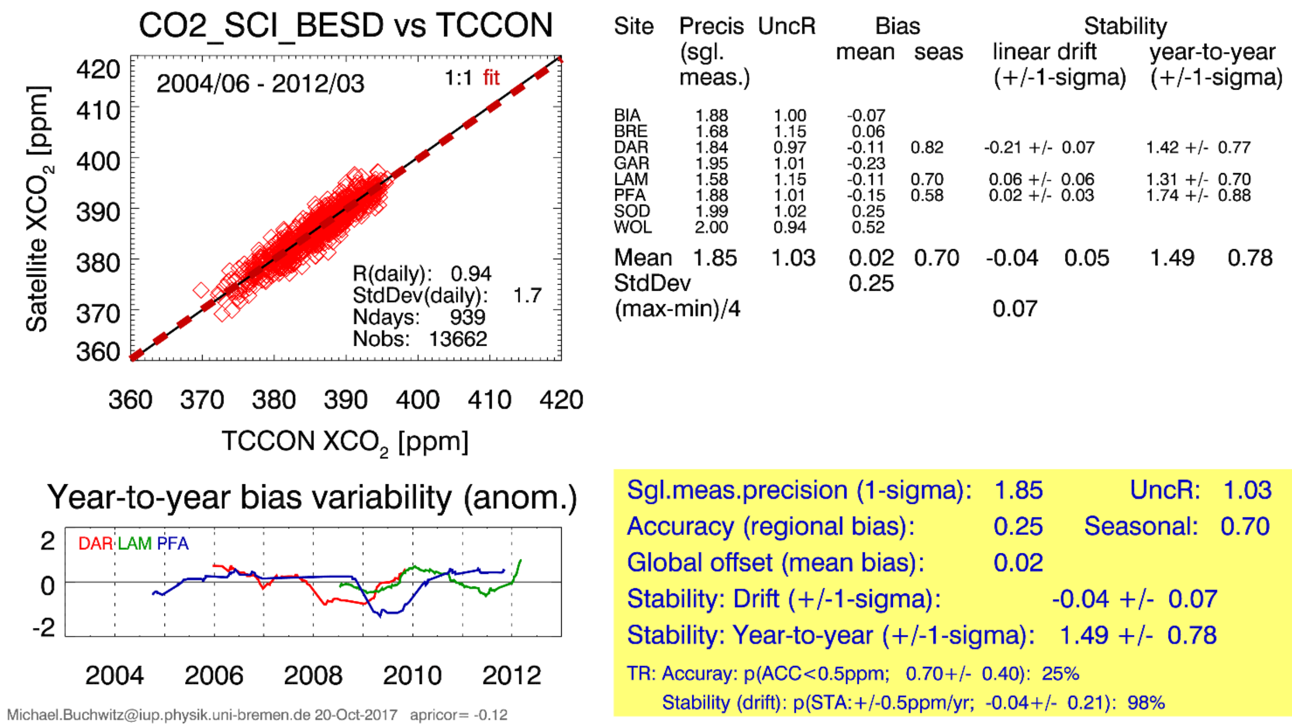


Table 6 - Product Quality Summary Table for product CO2_SCI_BESD as obtained by comparison with TCCON reference data. The listed requirements are the threshold (T) requirements as given in *TRD GHG, 2017*. For precision (i.e., single observation statistical uncertainty or random error) also the corresponding 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: 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	1.03	-	-	No requirement but value close to unity expected for a high quality data product.
Mean bias [ppm]	0.02	-	-	No requirement but value close to zero expected for a high quality data product.
Accuracy: Relative systematic error [ppm]	Spatial – spatiotemporal: 0.25 – 0.70	< 0.5	Probability that accuracy TR is met: 25%	-
Stability: Drift [ppm/year]	-0.04 +/- 0.07 (1-sigma)	< 0.5	Probability that stability TR is met: 98%	-
Stability: Year-to-year bias variability [ppm/year]	1.5 +/- 0.8 (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 7.

Figure 13 - As Figure 11 but for product CO2_SCI_WFMD.

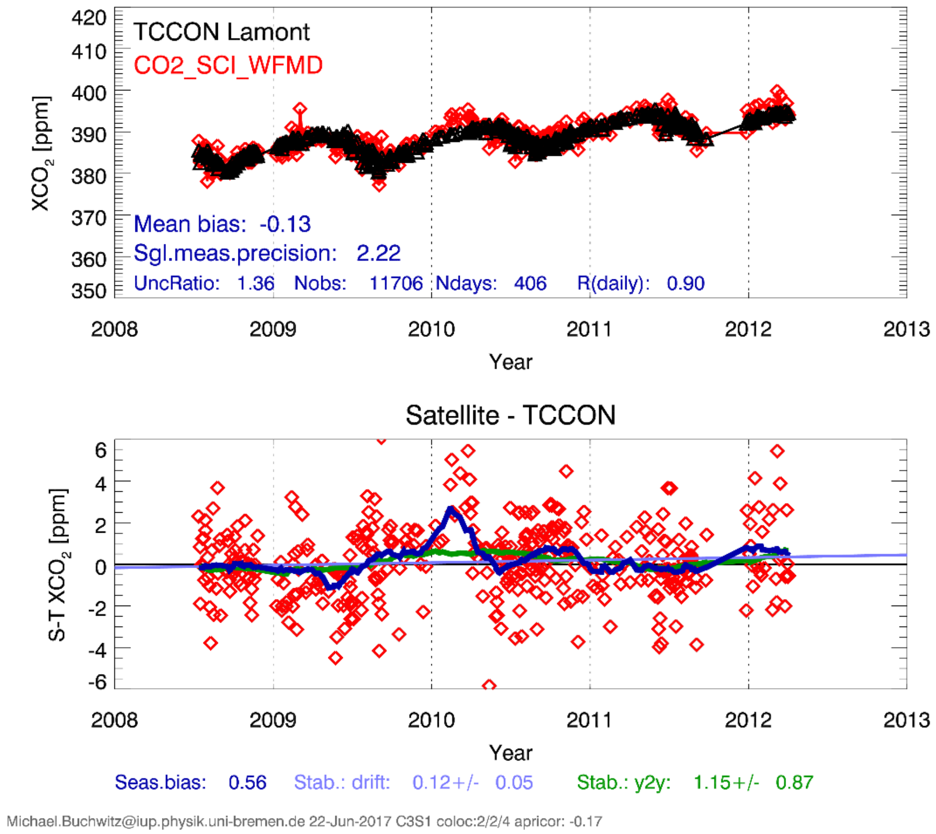


Figure 14 - As

Figure 12 but for product CO2_SCI_WFMD.

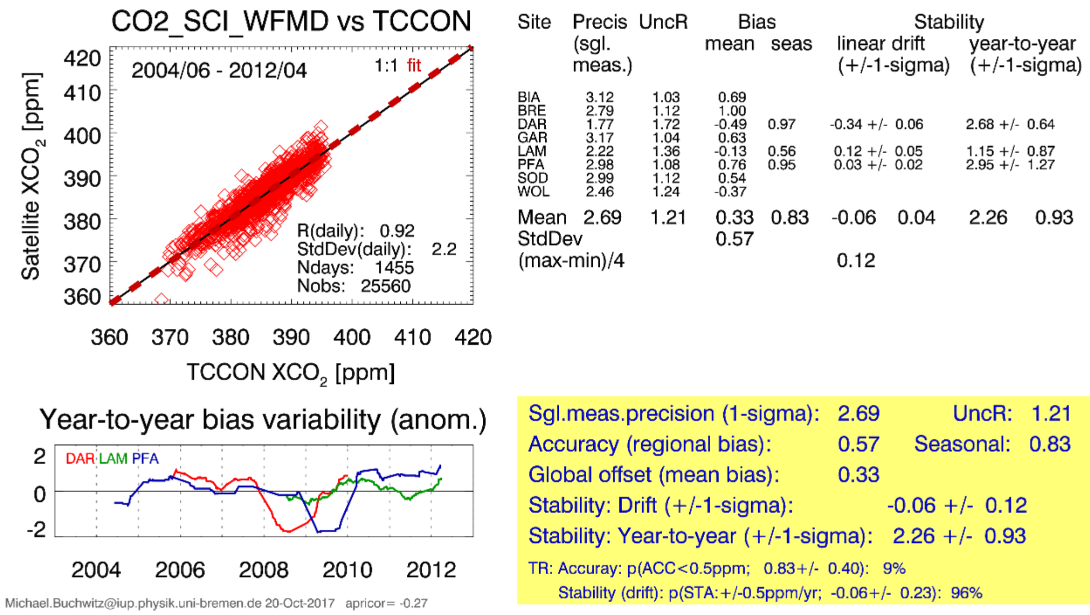


Table 7 - Product Quality Summary Table for product CO2_SCI_WFMD.

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	1.2	-	-	No requirement but value close to unity expected for a high quality data product.
Mean bias [ppm]	0.33	-	-	No requirement but value close to zero expected for a high quality data product.
Accuracy: Relative systematic error [ppm]	Spatial – spatiotemporal: 0.57 – 0.83	< 0.5	Probability that accuracy TR is met: 9%	-
Stability: Drift [ppm/year]	-0.06 +/- 0.12 (1-sigma)	< 0.5	Probability that stability TR is met: 96%	-
Stability: Year-to-year bias variability [ppm/year]	2.26 +/- 0.93 (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 7.

Figure 15 - As Figure 11 but for product CO2_GOS_OCFP.

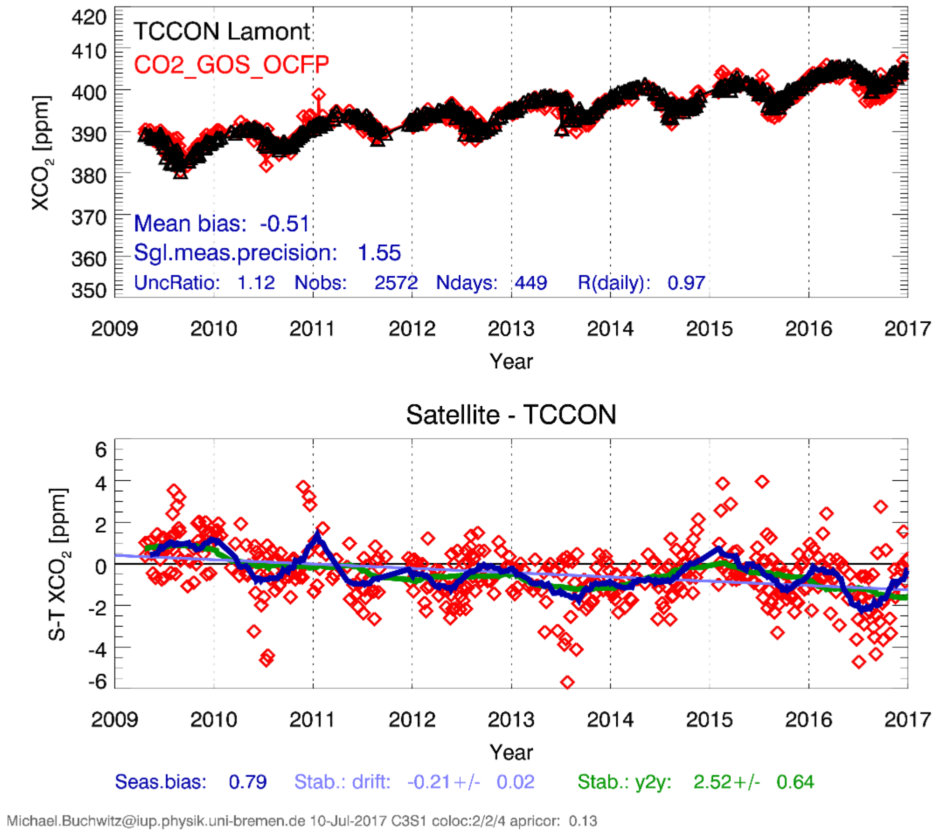


Figure 16 - As

Figure 12 but for product CO2_GOS_OCFP.

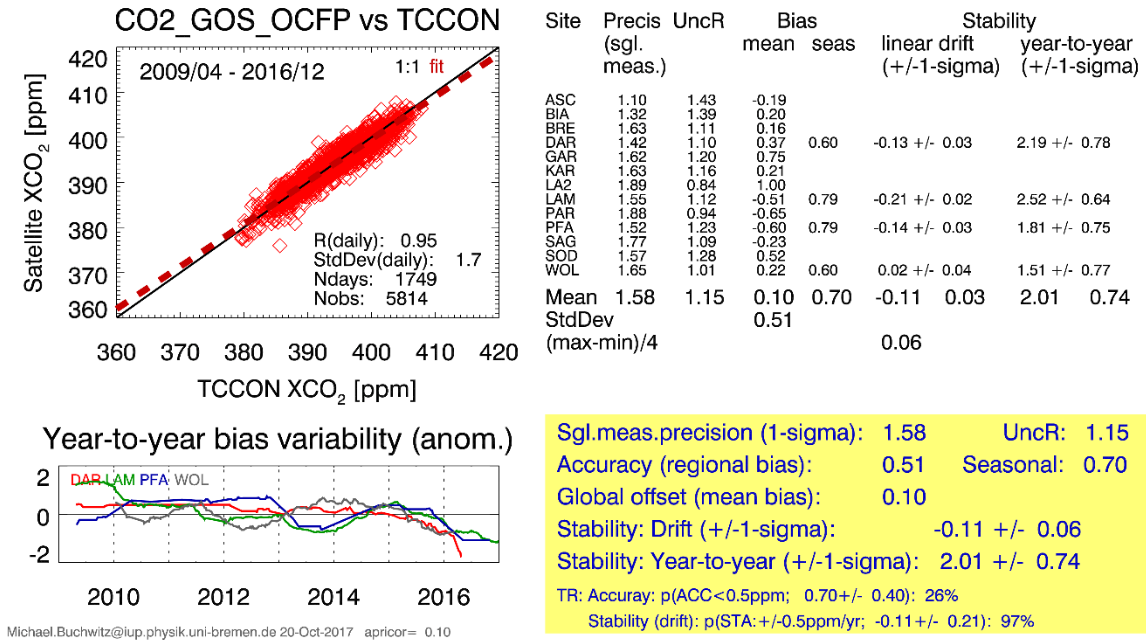


Table 8 - Product Quality Summary Table for product CO2_GOS_OCFP.

Product Quality Summary Table for Product: CO2_GOS_OCFP Level: 2, Version: 7.0, Time period covered: 4.2009 – 12.2016				
Parameter [unit]	Achieved performance	Requirement	TR	Comments
Single measurement precision (1-sigma) in [ppm]	1.6	< 8 (T) < 3 (B) < 1 (G)	-	-
Uncertainty ratio) in [-]: Ratio reported uncertainty to standard deviation of satellite-TCCON difference	1.15	-	-	No requirement but value close to unity expected for a high quality data product.
Mean bias [ppm]	0.10	-	-	No requirement but value close to zero expected for a high quality data product.
Accuracy: Relative systematic error [ppm]	Spatial – spatiotemporal: 0.51 – 0.70	< 0.5	Probability that accuracy TR is met: 26%	-
Stability: Drift [ppm/year]	-0.11 +/- 0.06 (1-sigma)	< 0.5	Probability that stability TR is met: 97%	-
Stability: Year-to-year bias variability [ppm/year]	2.01 +/- 0.74 (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 9.

Figure 17 - As Figure 11 but for product CO2_GOS_SRFP.

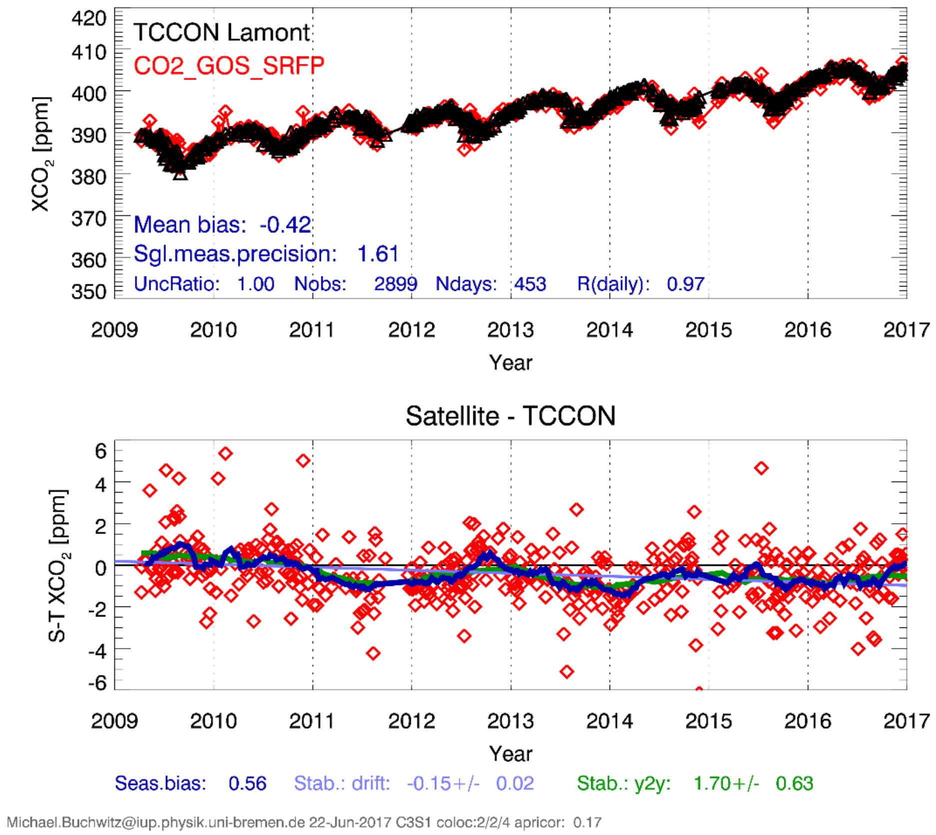


Figure 18 - As

Figure 12 but for product CO2_GOS_SRFP.

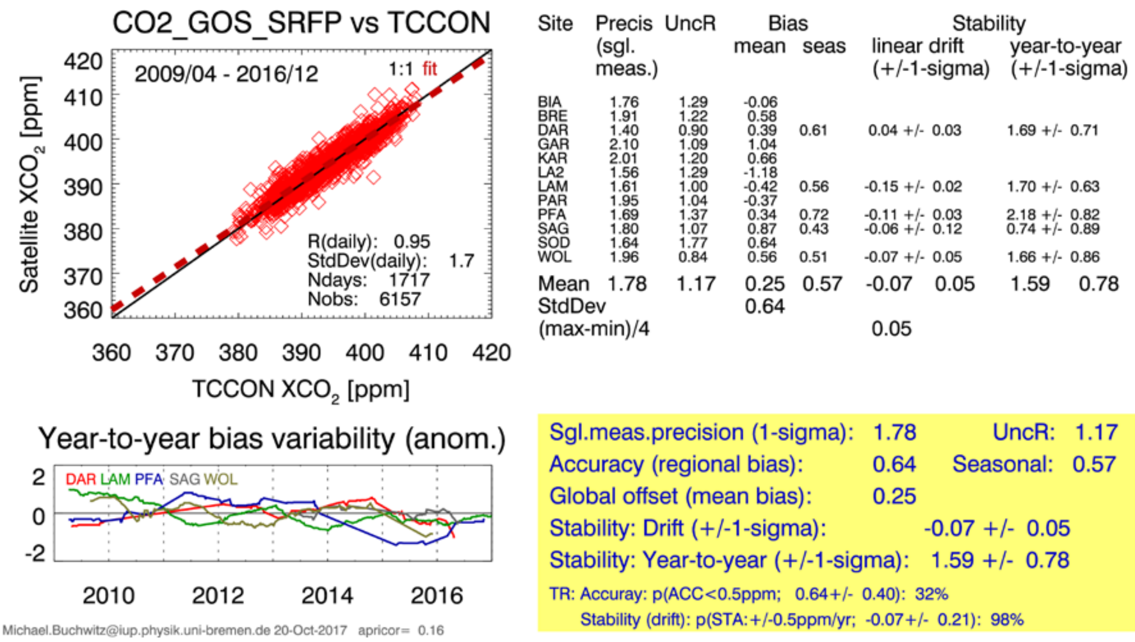


Table 9 - Product Quality Summary Table for product CO2_GOS_SRFP.

Product Quality Summary Table for Product: CO2_GOS_SRFP Level: 2, Version: 2.3.8, Time period covered: 6.2009 – 12.2016				
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	1.17	-	-	No requirement but value close to unity expected for a high quality data product.
Mean bias [ppm]	0.25	-	-	No requirement but value close to zero expected for a high quality data product.
Accuracy: Relative systematic error [ppm]	Spatial – spatiotemporal: 0.64 – 0.57	< 0.5	Probability that accuracy TR is met: 32%	-
Stability: Drift [ppm/year]	-0.07 +/- 0.05 (1-sigma)	< 0.5	Probability that stability TR is met: 98%	-
Stability: Year-to-year bias variability [ppm/year]	1.59 +/- 0.78 (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 9.

Figure 19 - As Figure 11 but for product XCO2_EMMA.

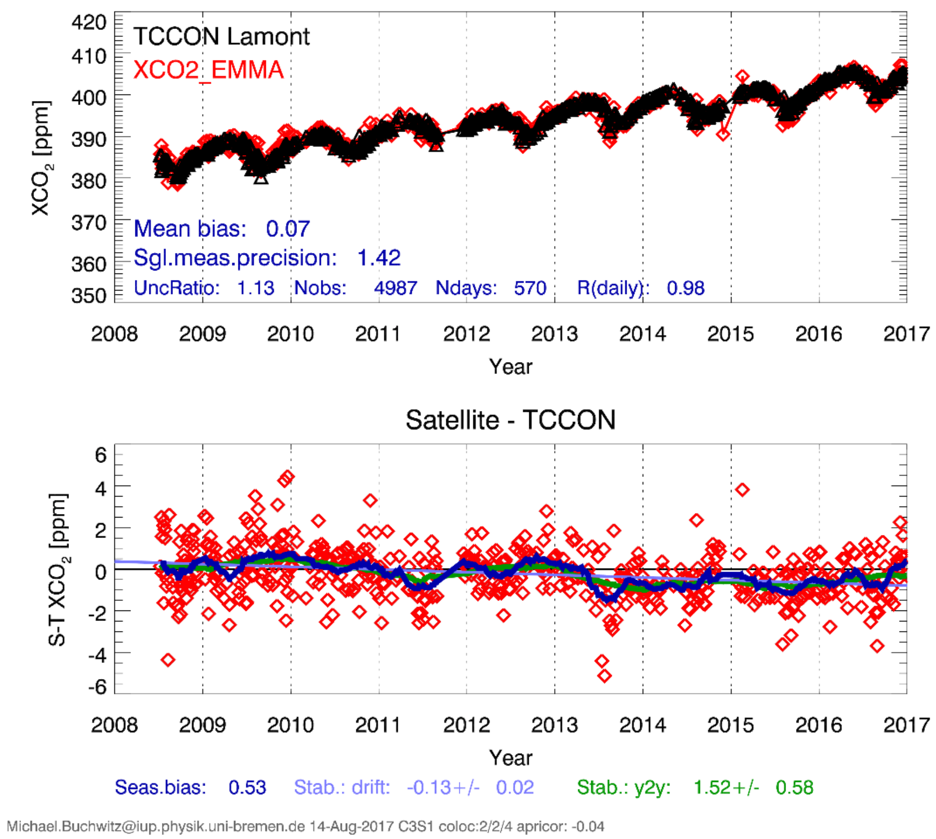


Figure 20 - As

Figure 12 but for product XCO2_EMMA.

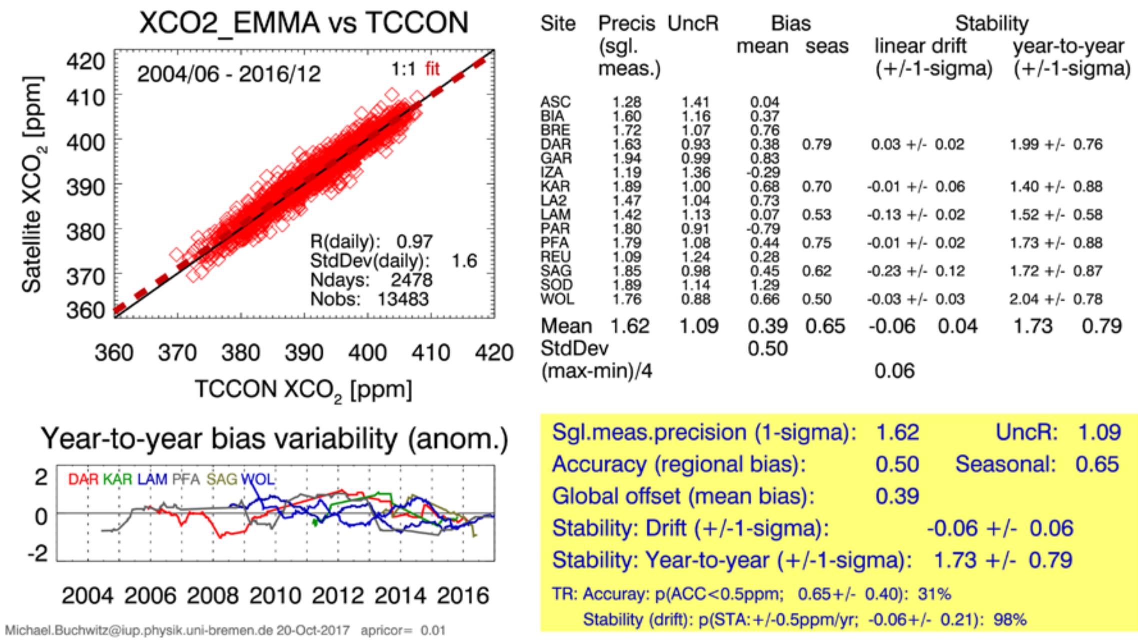


Table 10 - Product Quality Summary Table for product XCO2_EMMA.

Product Quality Summary Table for Product: XCO2_EMMA Level: 2, Version: 3.0, Time period covered: 1.2003 – 12.2016				
Parameter [unit]	Achieved performance	Requirement	TR	Comments
Single measurement precision (1-sigma) in [ppm]	1.62	< 8 (T) < 3 (B) < 1 (G)	-	-
Uncertainty ratio) in [-]: Ratio reported uncertainty to standard deviation of satellite-TCCON difference	1.09	-	-	No requirement but value close to unity expected for a high quality data product.
Mean bias [ppm]	0.39	-	-	No requirement but value close to zero expected for a high quality data product.
Accuracy: Relative systematic error [ppm]	Spatial – spatiotemporal: 0.50 – 0.65	< 0.5	Probability that accuracy TR is met: 31%	-
Stability: Drift [ppm/year]	-0.06 +/- 0.06 (1-sigma)	< 0.5	Probability that stability TR is met: 98%	-
Stability: Year-to-year bias variability [ppm/year]	1.73 +/- 0.79 (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 16 TCCON data set: Ascension, Bialystok, Bremen, Darwin, Garmisch, Izana, Karlsruhe, Lamont, Lauder 1 and 2, Paris, Park Falls, Reunion, Saga, Sodankyla, and Wollongong. Detailed information on each site can be found at https://tccon-wiki.caltech.edu/Sites. The used TCCON version is GGG2014 (data access: 22-June-2017).

Co-location criteria:

- Temporal: +/- 2 hours
- Spatial: +/- 2^o latitude, +/- 4^o 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 11.

Figure 21 - As Figure 11 but for product CH4_SCI_WFMD.

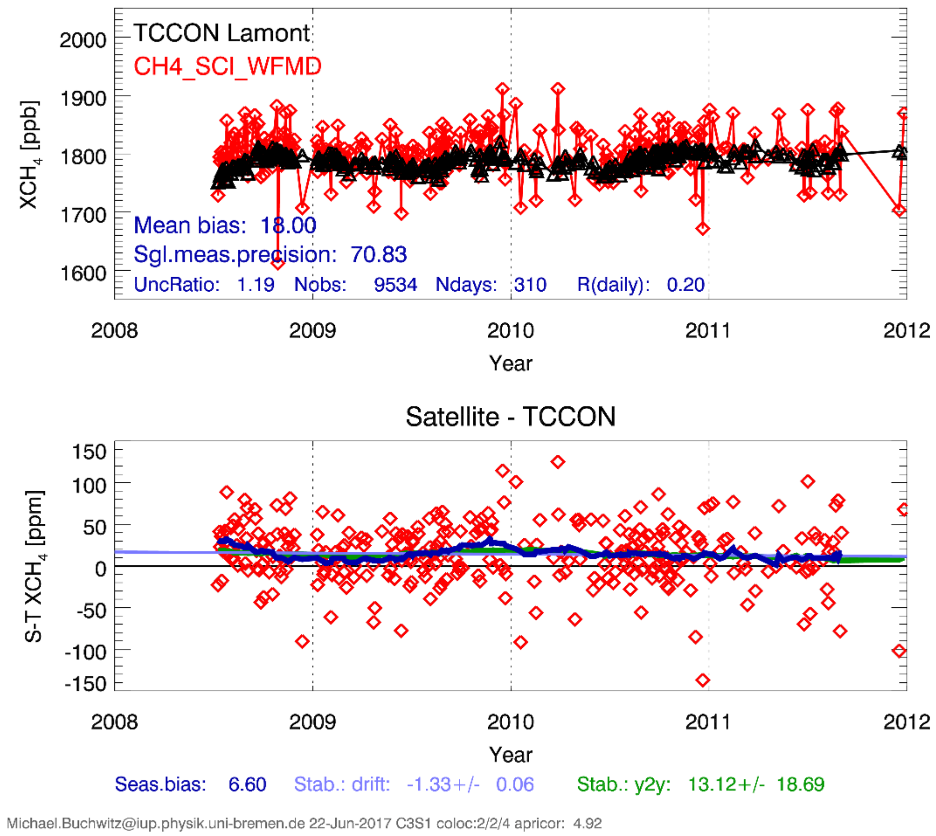


Figure 22 - As

Figure 12 but for product CH4_SCI_WFMD.

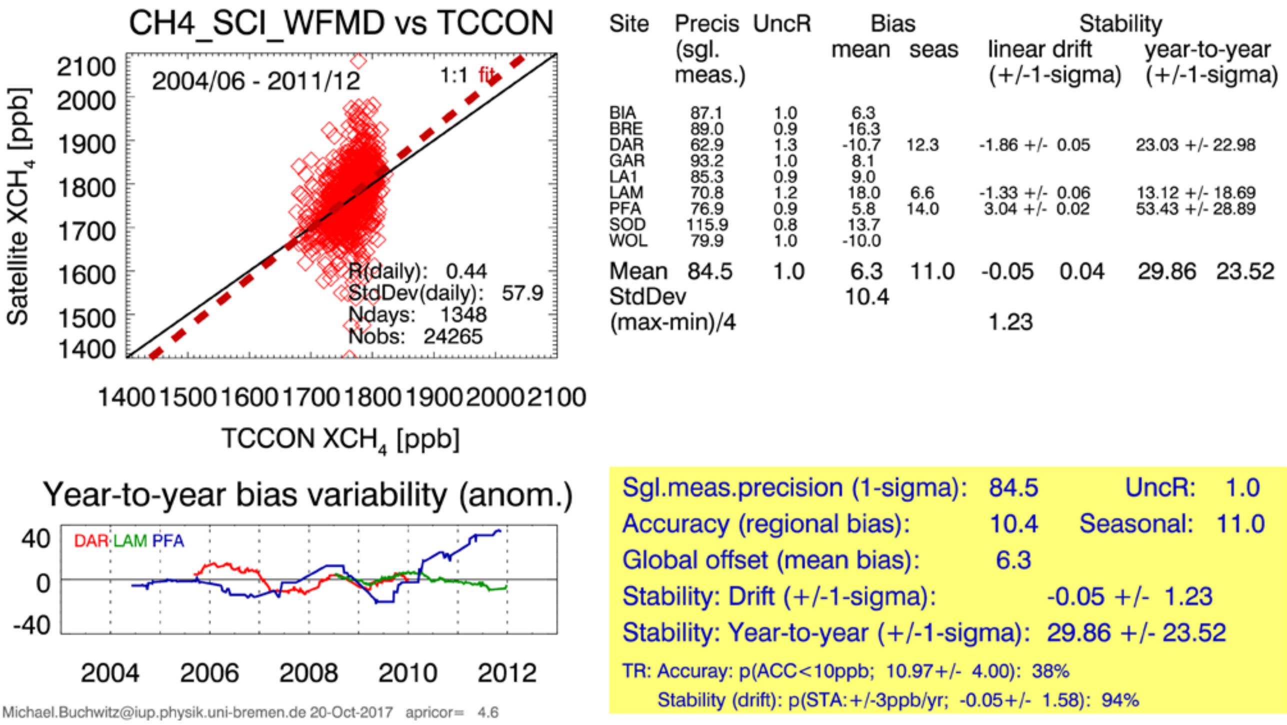


Table 11 - Product Quality Summary Table for product CH4_SCI_WFMB as obtained by comparison with TCCON reference data. The listed requirements are the threshold (T) requirements as given in *TRD GHG, 2017*. For precision (i.e., single observation statistical uncertainty or random error) also the corresponding 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]	85	< 34 (T) < 17 (B) < 9 (G)	-	-
Uncertainty ratio) in [-]: Ratio reported uncertainty to standard deviation of satellite-TCCON difference	1.0	-	-	No requirement but value close to unity expected for a high quality data product.
Mean bias [ppb]	6.3	-	-	No requirement but value close to zero expected for a high quality data product.
Accuracy: Relative systematic error [ppb]	Spatial – spatiotemporal: 10.4 – 11.0	< 10	Probability that accuracy TR is met: 38%	-
Stability: Linear bias trend [ppb/year]	-0.05 +/- 1.23 (1-sigma)	< 3	Probability that stability TR is met: 94%	-
Stability: Year-to-year bias variability [ppb/year]	30 +/- 24 (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 12.

Figure 23 - As Figure 11 but for product CH4_SCI_IMAP.

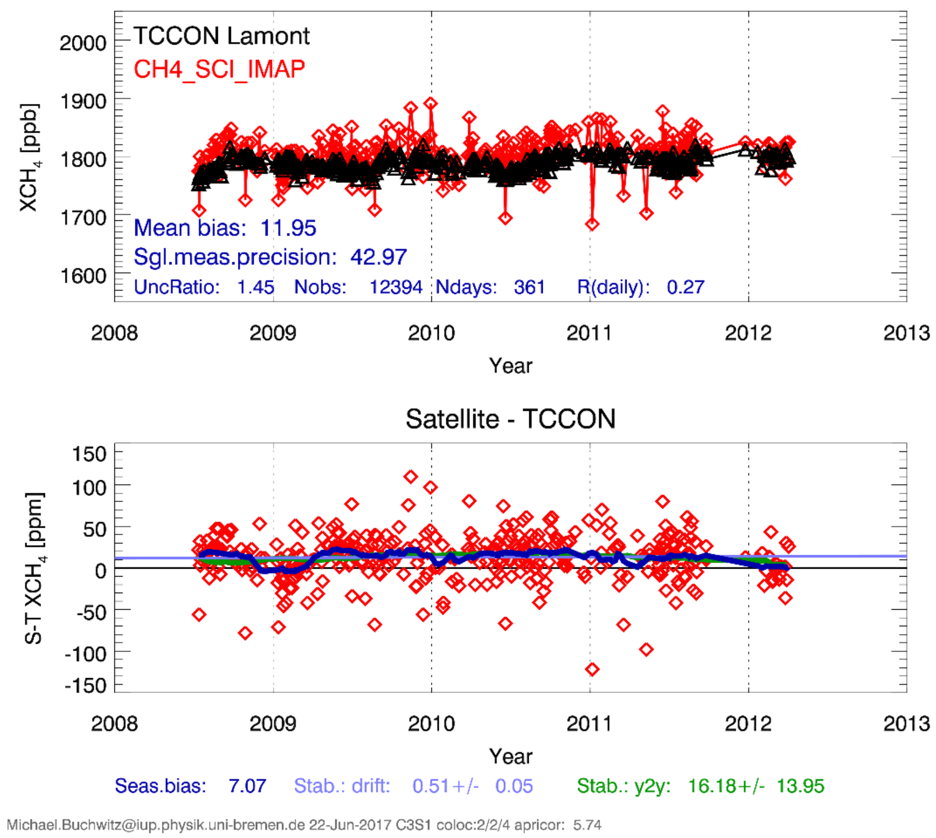


Figure 24 - As

Figure 12 but for product CH4_SCI_IMAP.

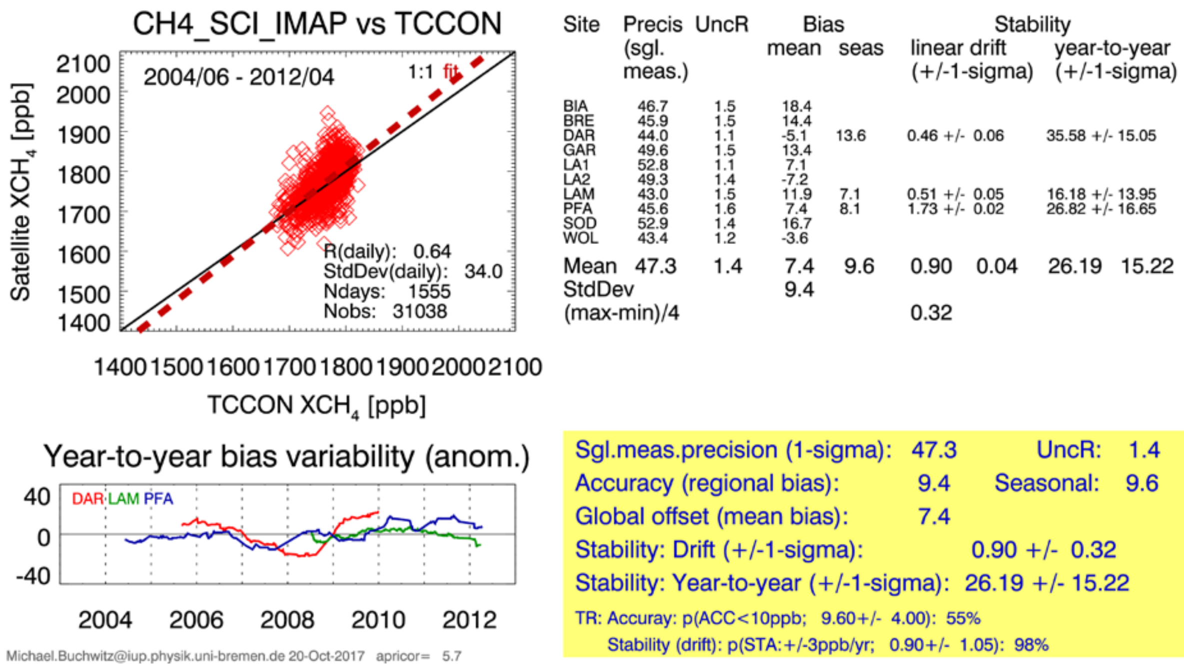


Table 12 - Product Quality Summary Table for product CH4_SCI_IMAP.

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	1.4	-	-	No requirement but value close to unity expected for a high quality data product.
Mean bias [ppb]	7.4	-	-	No requirement but value close to zero expected for a high quality data product.
Accuracy: Relative systematic error [ppb]	Spatial – spatiotemporal: 9.4 – 9.6	< 10	Probability that accuracy TR is met: 55%	-
Stability: Linear bias trend [ppb/year]	0.90 +/- 0.32 (1-sigma)	< 3	Probability that stability TR is met: 98%	-
Stability: Year-to-year bias variability [ppb/year]	26 +/- 15 (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 13.

Figure 25 - As Figure 11 but for product CH4_GOS_OCPR.

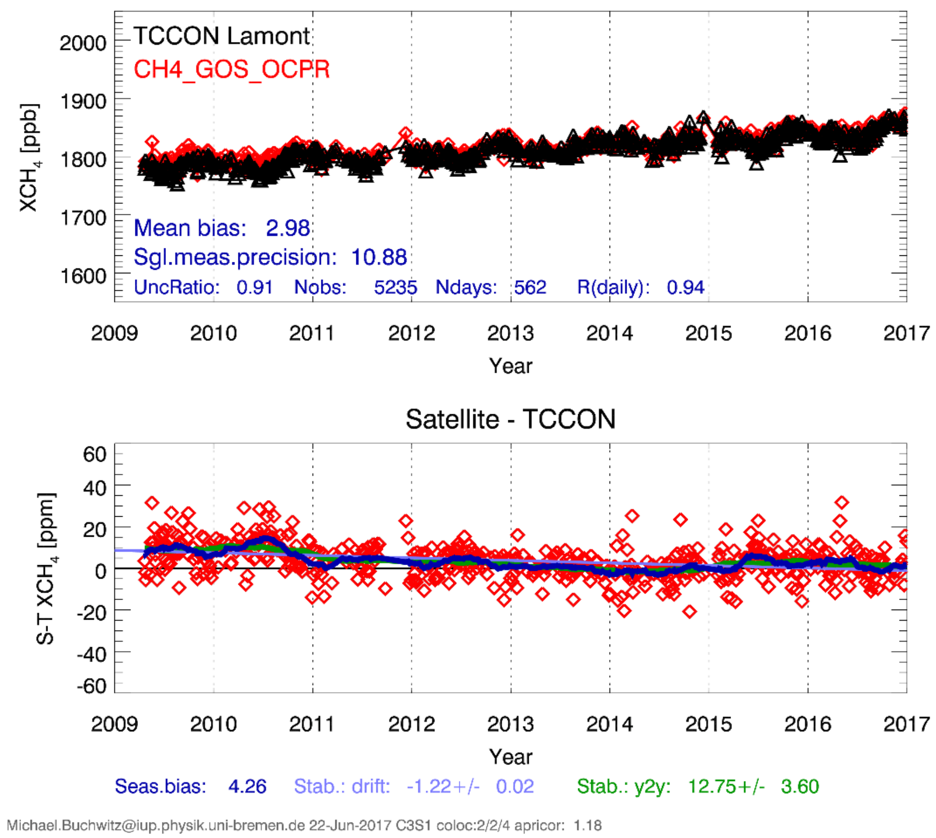


Figure 26 - As

Figure 12 but for product CH4_GOS_OCPR.

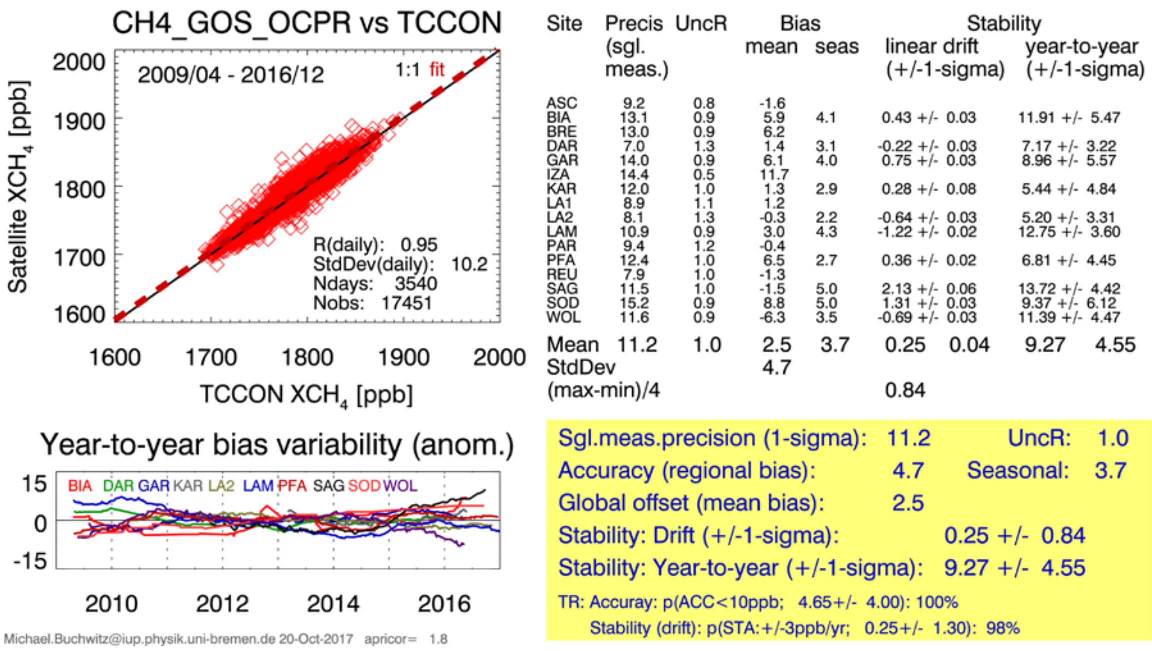


Table 13 - Product Quality Summary Table for product CH4_GOS_OCPR.

Product Quality Summary Table for Product: CH4_GOS_OCPR Level: 2, Version: 7.0, Time period covered: 4.2009 – 12.2016				
Parameter [unit]	Achieved performance	Requirement	TR	Comments
Single measurement precision (1-sigma) in [ppb]	11	< 34 (T) < 17 (B) < 9 (G)	-	-
Uncertainty ratio) in [-]: Ratio reported uncertainty to standard deviation of satellite-TCCON difference	1.0	-	-	No requirement but value close to unity expected for a high quality data product.
Mean bias [ppb]	2.5	-	-	No requirement but value close to zero expected for a high quality data product.
Accuracy: Relative systematic error [ppb]	Spatial – spatiotemporal: 4.7 – 3.7	< 10	Probability that accuracy TR is met: 100%	-
Stability: Linear bias trend [ppb/year]	0.25 +/- 0.84 (1-sigma)	< 3	Probability that stability TR is met: 98%	-
Stability: Year-to-year bias variability [ppb/year]	9.3 +/- 4.6 (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 14.

Figure 27 - As Figure 11 but for product CH4_GOS_SRPR.

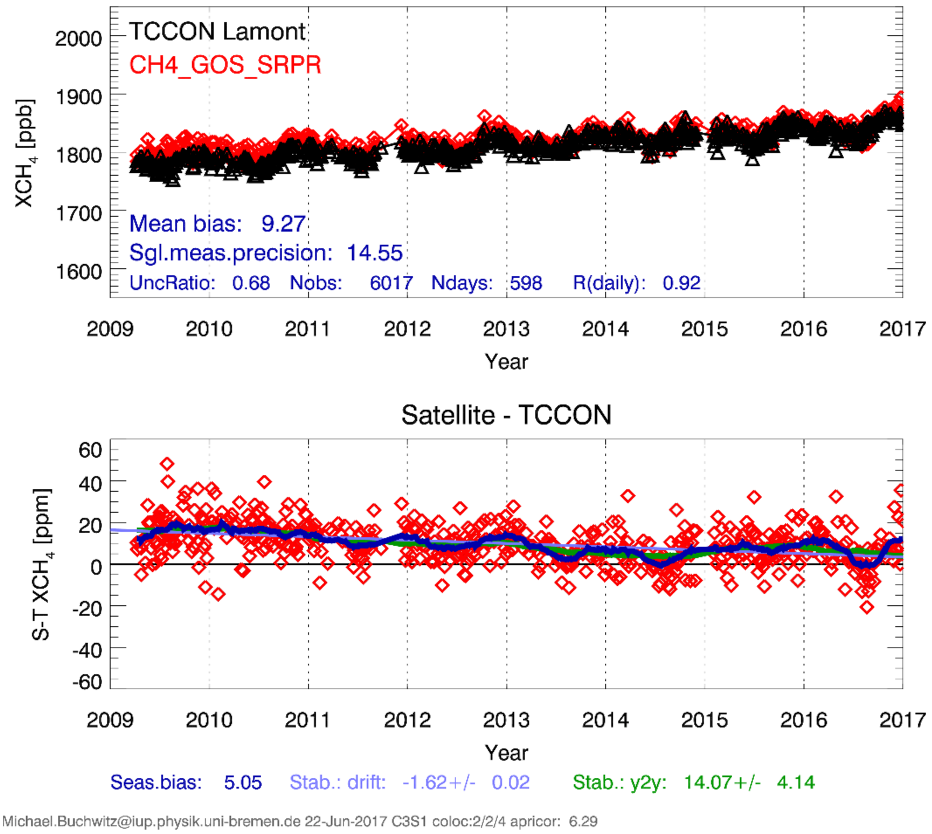


Figure 28 - As

Figure 12 but for product CH4_GOS_SRPR.

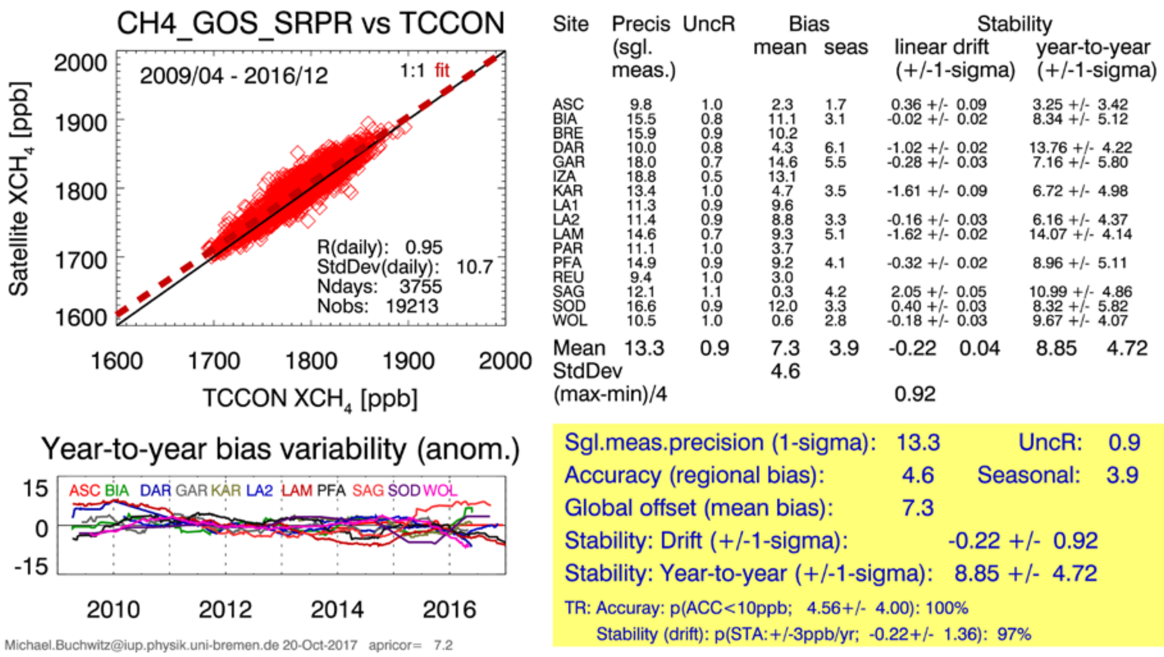


Table 14 - Product Quality Summary Table for product CH4_GOS_SRPR.

Product Quality Summary Table for Product: CH4_GOS_SRPR Level: 2, Version: 2.3.8, Time period covered: 6.2009 – 12.2016				
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	0.9	-	-	No requirement but value close to unity expected for a high quality data product.
Mean bias [ppb]	7.3	-	-	No requirement but value close to zero expected for a high quality data product.
Accuracy: Relative systematic error [ppb]	Spatial – spatiotemporal: 4.9 – 3.9	< 10	Probability that accuracy TR is met: 100%	-
Stability: Linear bias trend [ppb/year]	-0.22 +/- 0.92 (1-sigma)	< 3	Probability that stability TR is met: 97%	-
Stability: Year-to-year bias variability [ppb/year]	8.9 +/- 4.7 (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 15.

Figure 29 - As Figure 11 but for product CH4_GOS_OCFP.

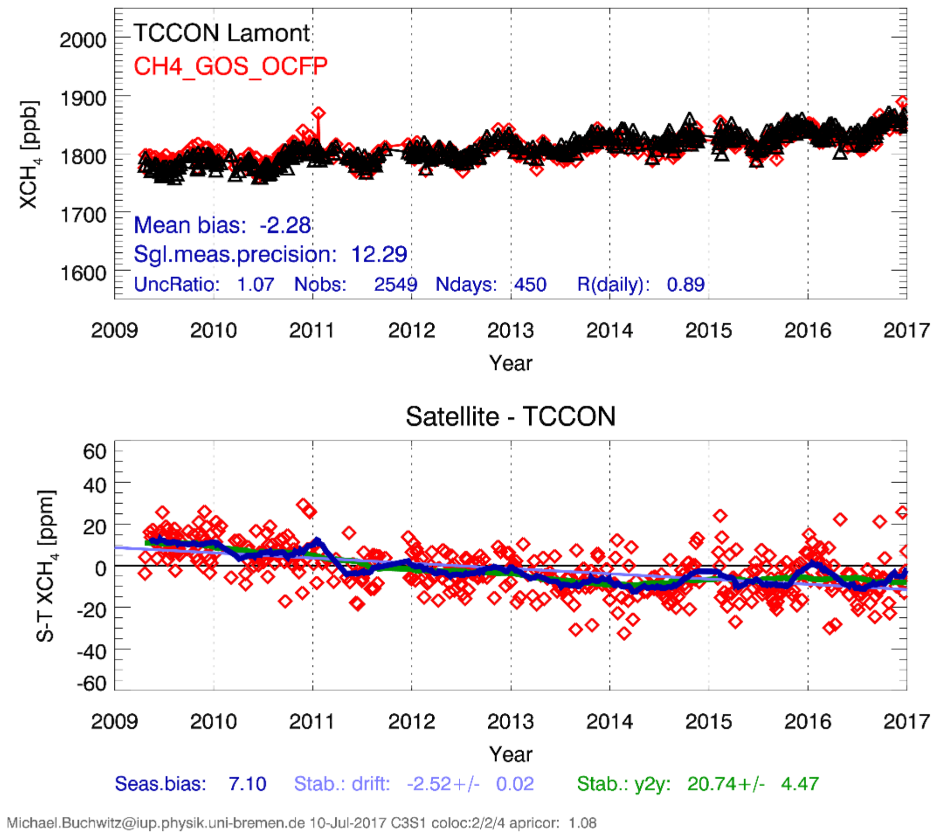


Figure 30 - As

Figure 12 but for product CH4_GOS_OCFP.

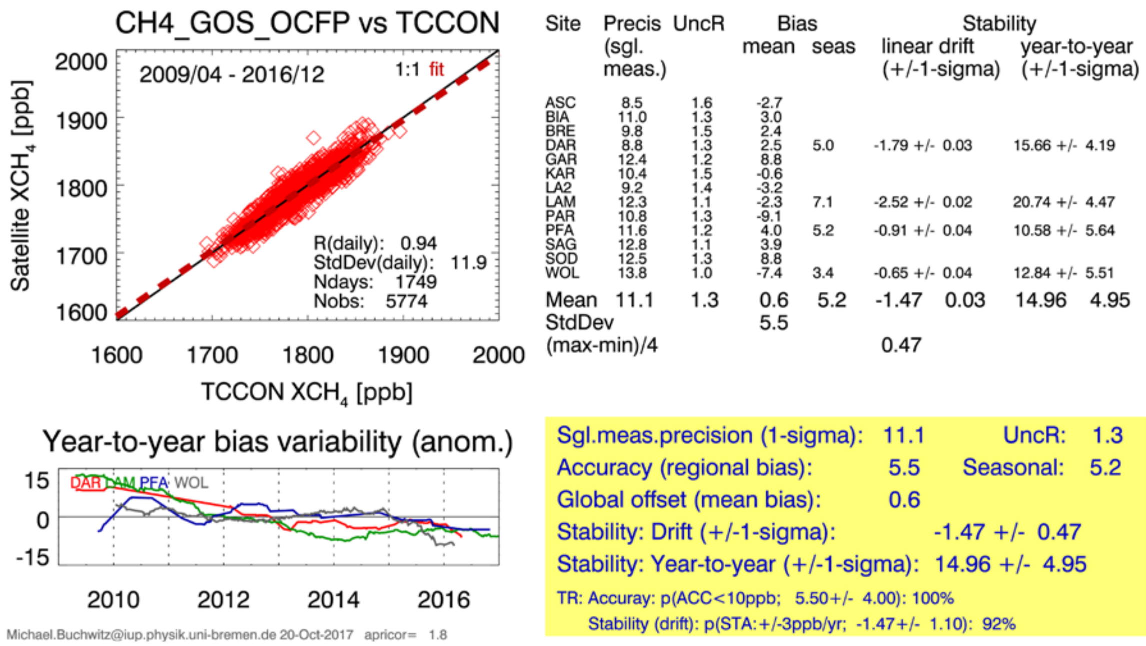


Table 15 - Product Quality Summary Table for product CH4_GOS_OCFP.

Product Quality Summary Table for Product: CH4_GOS_OCFP Level: 2, Version: 2.02, Time period covered: 4.2009 – 12.2016				
Parameter [unit]	Achieved performance	Requirement	TR	Comments
Single measurement precision (1-sigma) in [ppb]	11	< 34 (T) < 17 (B) < 9 (G)	-	-
Uncertainty ratio) in [-]: Ratio reported uncertainty to standard deviation of satellite-TCCON difference	1.3	-	-	No requirement but value close to unity expected for a high quality data product.
Mean bias [ppb]	0.6	-	-	No requirement but value close to zero expected for a high quality data product.
Accuracy: Relative systematic error [ppb]	Spatial – spatiotemporal: 5.5 – 5.2	< 10	Probability that accuracy TR is met: 100%	-
Stability: Linear bias trend [ppb/year]	-1.5 +/- 0.5 (1-sigma)	< 3	Probability that stability TR is met: 92%	-
Stability: Year-to-year bias variability [ppb/year]	15 +/- 5 (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 16.

Figure 31 - As Figure 11 but for product CH4_GOS_SRFP.

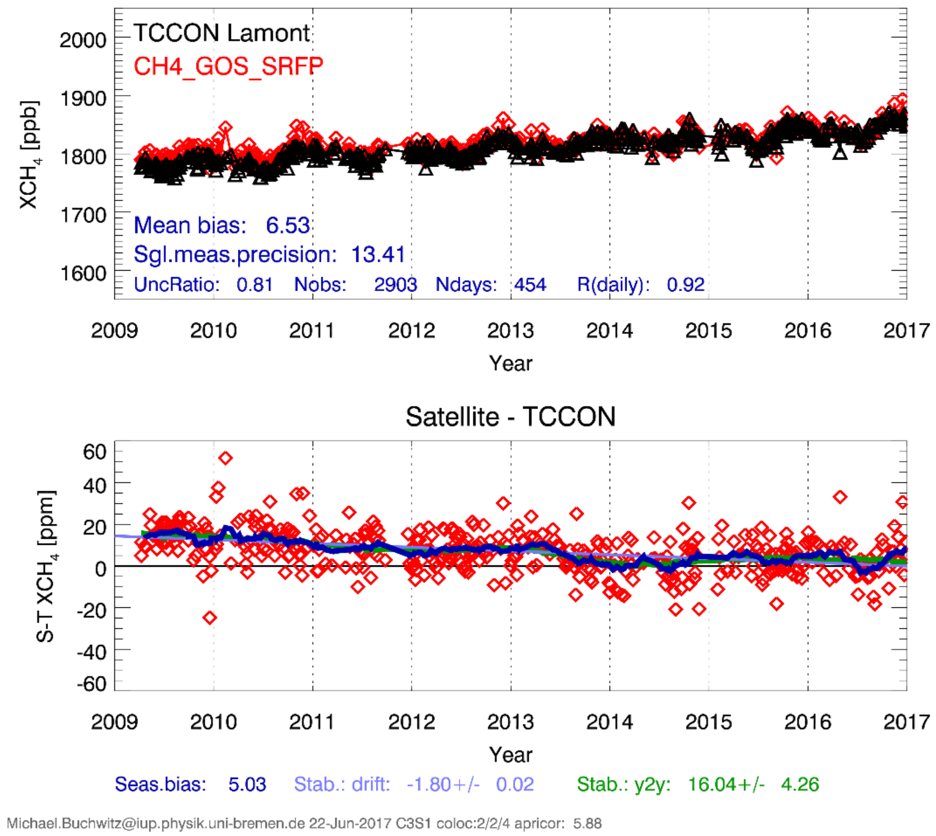


Figure 32 – As

Figure 12 but for product CH4_GOS_SRFP.

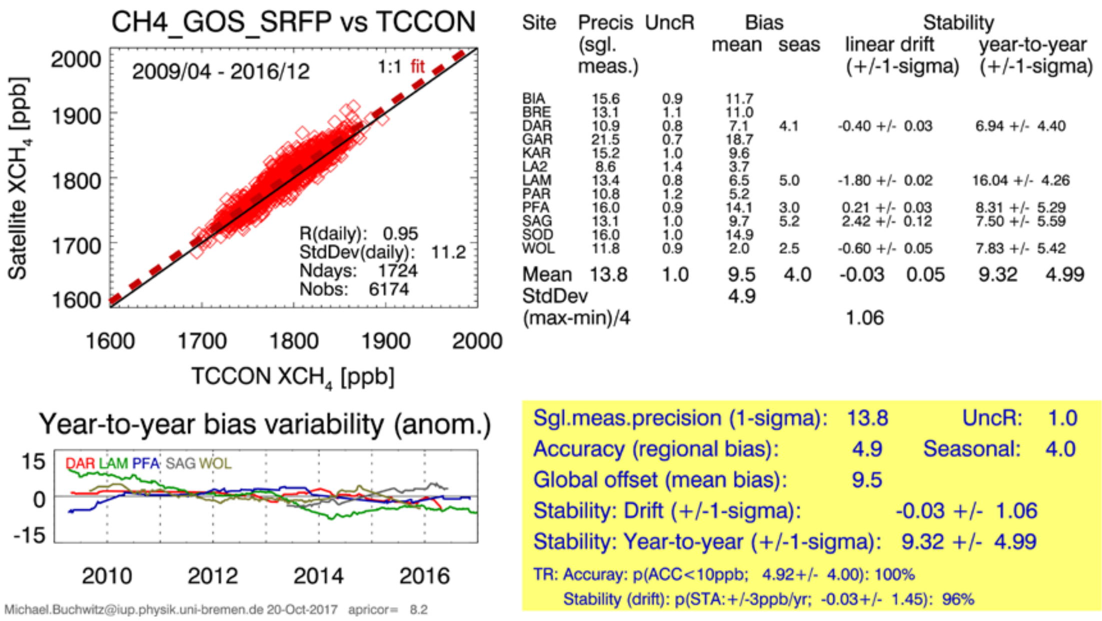


Table 16 - Product Quality Summary Table for product CH4_GOS_SRFP.

Product Quality Summary Table for Product: CH4_GOS_SRFP Level: 2, Version: 2.3.8, Time period covered: 6.2009 – 12.2016				
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	1.0	-	-	No requirement but value close to unity expected for a high quality data product.
Mean bias [ppb]	9.5	-	-	No requirement but value close to zero expected for a high quality data product.
Accuracy: Relative systematic error [ppb]	Spatial – spatiotemporal: 4.9 – 4.0	< 10	Probability that accuracy TR is met: 100%	-
Stability: Linear bias trend [ppb/year]	-0.03 +/- 1.06 (1-sigma)	< 3	Probability that stability TR is met: 96%	-
Stability: Year-to-year bias variability [ppb/year]	9.3 +/- 5.0 (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 16.

Figure 33 - As Figure 11 but for product CH4_GOS_SRFP. The large scatter before mid 2009 is due to the worse performance of SCIAMACHY compared to GOSAT.

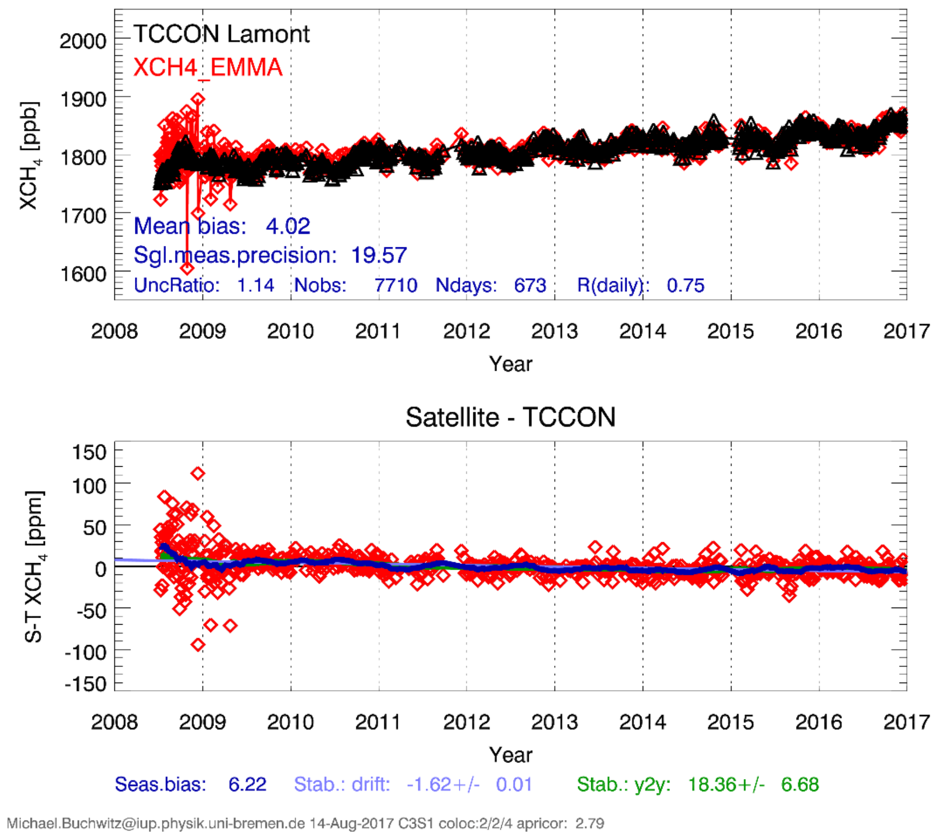


Figure 34 – As

Figure 12 but for product XCH4_EMMA. The “outliers” are due to SCIAMACHY only data before mid 2009.

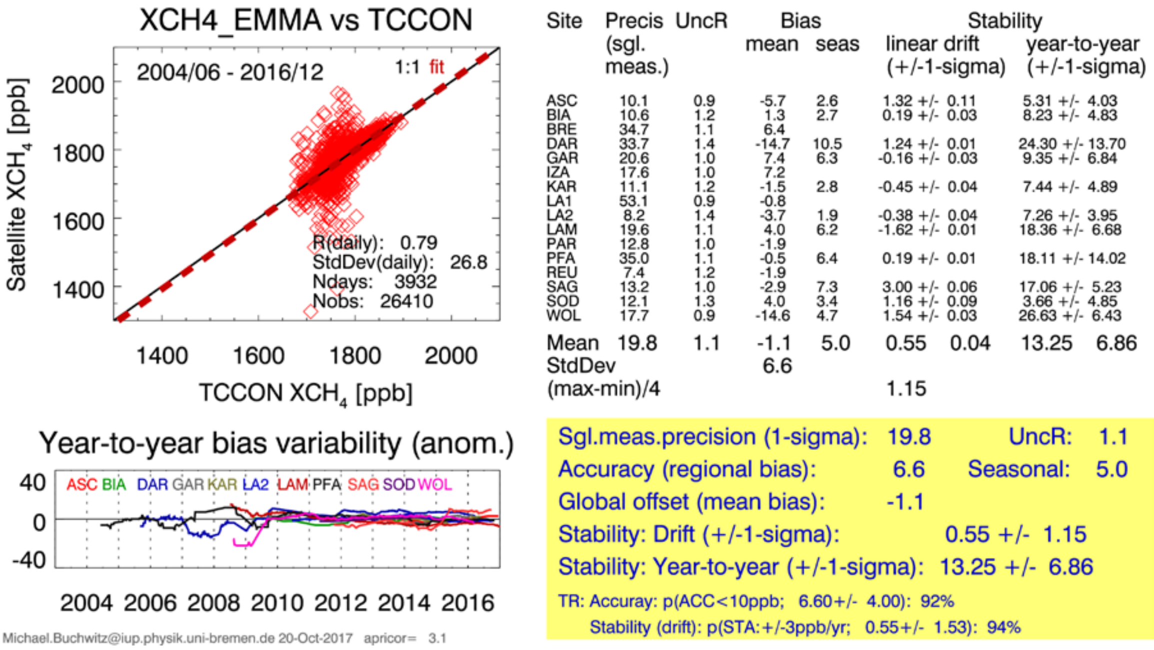


Table 17 - Product Quality Summary Table for product XCH4_EMMA.

Product Quality Summary Table for Product: XCH4_EMMA Level: 2, Version: 3.0, Time period covered: 1.2003 – 12.2016				
Parameter [unit]	Achieved performance	Requirement	TR	Comments
Single measurement precision (1-sigma) in [ppb]	19.8	< 34 (T) < 17 (B) < 9 (G)	-	-
Uncertainty ratio) in [-]: Ratio reported uncertainty to standard deviation of satellite-TCCON difference	1.1	-	-	No requirement but value close to unity expected for a high quality data product.
Mean bias [ppb]	-1.1	-	-	No requirement but value close to zero expected for a high quality data product.
Accuracy: Relative systematic error [ppb]	Spatial – spatiotemporal: 6.6 – 5.0	< 10	Probability that accuracy TR is met: 92%	-
Stability: Linear bias trend [ppb/year]	0.55 +/- 1.15 (1-sigma)	< 3	Probability that stability TR is met: 94%	-
Stability: Year-to-year bias variability [ppb/year]	13.25 +/- 6.86 (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 as for the Level 2 products but with the following exceptions:

- The (monthly mean) product has been compared with monthly mean TCCON data not considering averaging kernels.
- The “single measurement precision” is not part of this product and therefore has not been validated and for the same reason this is also true for the reported uncertainty.
- Seasonal biases have not been used for accuracy and stability assessments because at maximum only 3 data points are available per season.

Figure 35 shows the comparison at the TCCON site Lamont, Oklahoma, USA, and Figure 36 shows an overview about all validation results.

Table 18 shows the product quality summary table for this product.

Figure 35 – As Figure 11 but for product XCO2_OBS4MIPS. Note that this product has been generated quasi automatically using a well defined procedure. Potential outliers, such as the one in the first half of 2008, have not been removed “by hand”.

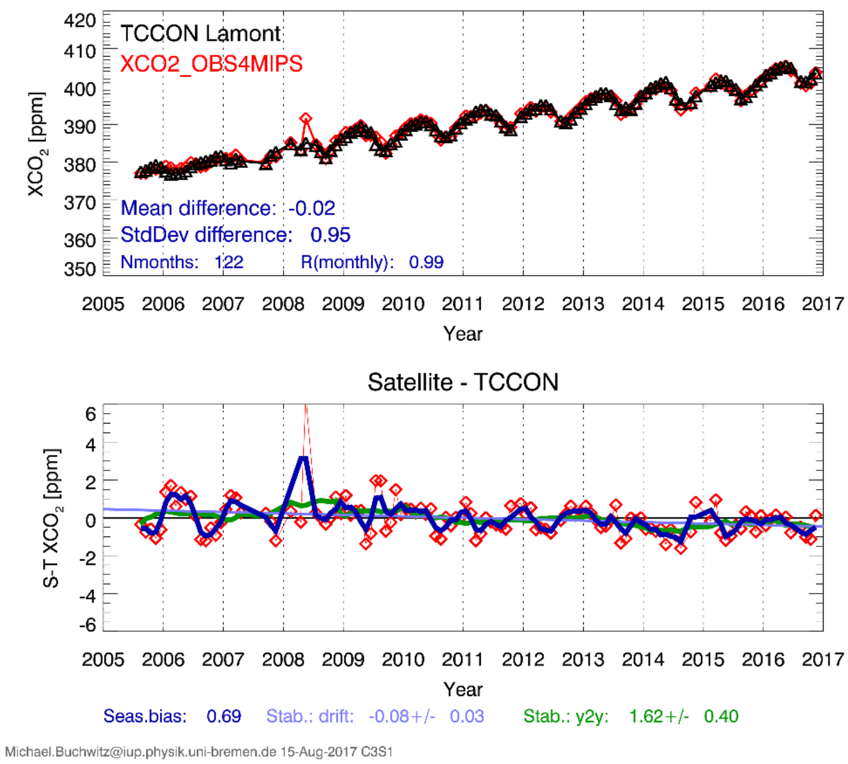


Figure 36 – Similar as Figure 12 but for product XCO2_OBS4MIPS.

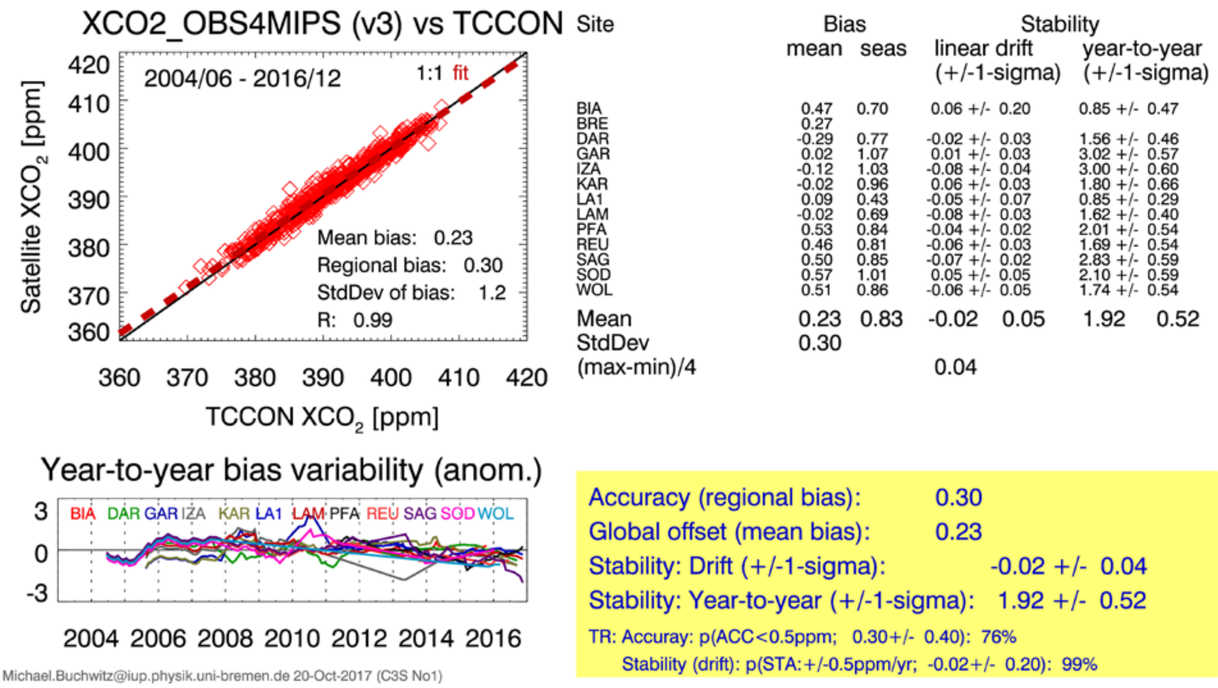


Table 18 – Product Quality Summary Table for product XCO2_OBS4MIPS.

Product Quality Summary Table for Product: XCO2_OBS4MIPS Level: 3, Version: 3, Time period covered: 1.2003 – 12.2016				
Parameter [unit]	Achieved performance	Requirement	TR	Comments
Mean bias [ppm]	0.23	-	-	No requirement but value close to zero expected for a high quality data product.
Accuracy: Relative systematic error [ppm]	Regional bias: 0.30	< 0.5	Probability that accuracy TR is met: 76%	-
Stability: Linear bias trend [ppm/year]	-0.02 +/- 0.04 (1-sigma)	< 0.5	Probability that stability TR is met: 99%	-
Stability: Year-to-year bias variability [ppm/year]	1.92 +/- 0.52 (1-sigma)	< 0.5	-	-

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 as for the Level 2 products but with the following exceptions:

- The (monthly mean) product has been compared with monthly mean TCCON data not considering averaging kernels.
- The "single measurement precision" is not part of this product and therefore has not been validated and for the same reason this is also true for the reported uncertainty.
- Seasonal biases have not been used for accuracy and stability assessments because at maximum only 3 data points are available per season.

Figure 37 shows the comparison at the TCCON site Lamont, Oklahoma, USA, and Figure 38 shows an overview about all validation results.

Table 19 shows the product quality summary table for this product.

Figure 37 – As Figure 11 but for product XCH4_OBS4MIPS.

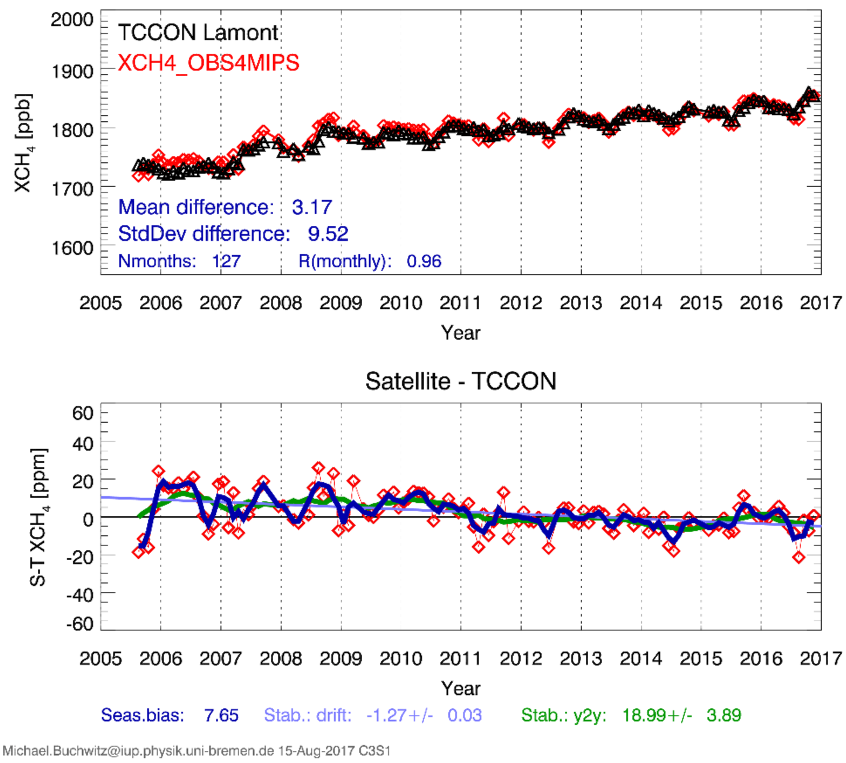


Figure 38 – Similar as Figure 12 but for product XCH4_OBS4MIPS.

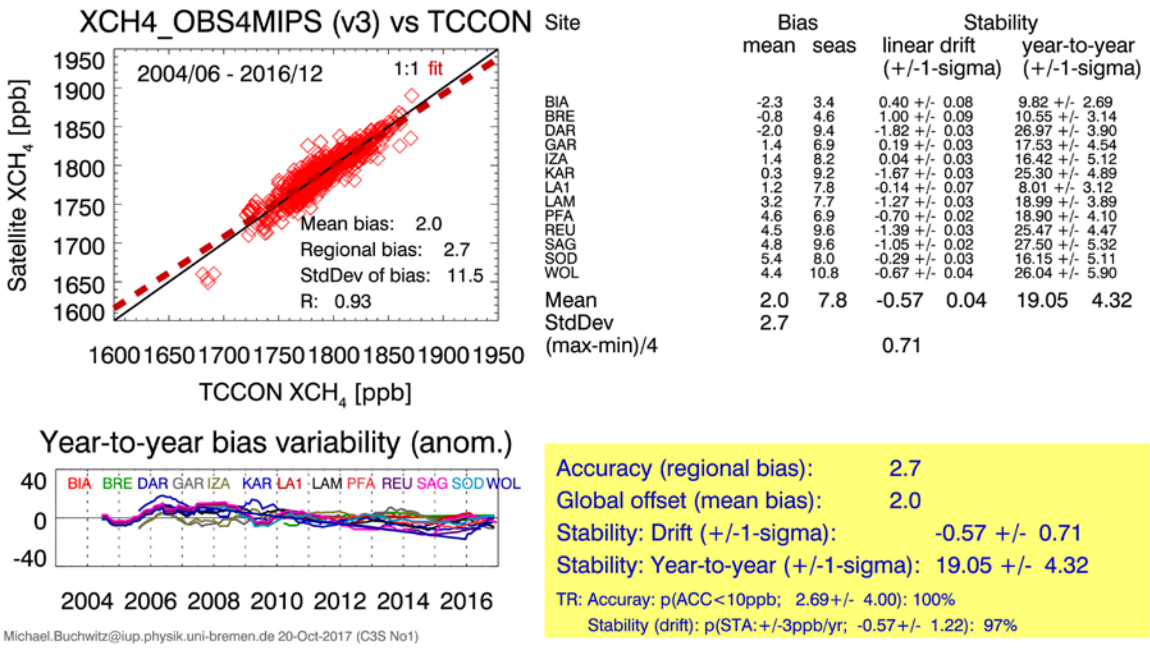


Table 19 – Product Quality Summary Table for product XCH4_OBS4MIPS.

Product Quality Summary Table for Product: XCH4_OBS4MIPS Level: 3, Version: 3, Time period covered: 1.2003 – 12.2016				
Parameter [unit]	**Achieved performance**	**Requirement**	**TR**	**Comments**
Mean bias [ppb]	2.0	-	-	No requirement but value close to zero expected for a high quality data product.
Accuracy: Relative systematic error [ppb]	Regional bias: 2.7	< 10	Probability that accuracy TR is met: 100%	-
Stability: Linear bias trend [ppb/year]	-0.57 +/- 0.71 (1-sigma)	< 3	Probability that stability TR is met: 97%	-
Stability: Year-to-year bias variability [ppb/year]	19.05 +/- 4.3 (1-sigma)	< 3	-	-

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 20 - Table 22.

As shown in Annex E, the IASI and AIRS observations were spatially and temporally collocated with observations made from aircraft measurements from the CONTRAIL and HIPPO programs, as well as with observations made from balloons using AirCores. When enough in-situ data were available, a number of statistics, including accuracy and stability, have been computed from the difference between in-situ measurements and retrievals from space observation.

Overall, the CNRS-LMD products are found to be highly stable and appear to meet the TR requirements for accuracy and stability, especially for the products from IASI on Metop-A. For IASI on Metop-B investigations were limited by lack of reference data are. Product CO2_IASB_NLIS (Metop-B) has a low bias of about 2 ppm compared to product CO2_IASA_NLIS (Metop-A).

It has to be noted that, due to too sparse validation data for CH_4, the TR for stability could not be computed. This calls for continuous effort in performing and developing continuous airborne observations of greenhouse gases.

Table 20 - Product Quality Summary Table for product CO2_IASA_NLIS.

Product Quality Summary Table for Product: CO2_IASA_NLIS Level: 2, Version: 7.0, Time period covered: 4.2009 – 12.2015				
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]	0.57	-	-	No requirement but value close to zero expected for a high quality data product.
Accuracy: Relative systematic error [ppm]	Spatial – spatiotemporal: 0.46 / 0.49	< 0.5	Probability that accuracy TR is met: 100%	-
Stability: Drift [ppm/year]	-0.01 ± 0.01 (1-sigma)	< 0.5	Probability that stability TR is met: 100%	-
Stability: Year-to-year bias variability [ppm/year]	2.64 ± 0.79 (1-sigma)	< 0.5	-	-

Table 21 - Product Quality Summary Table for products CH4_IASA_NLIS (NC stands for Not computed due to lack of available data).

<table>
<tr><td colspan="5">Product Quality Summary Table for Product: CH4_IASA_NLIS
Level: 2, Version: 7.0, Time period covered: 4.2009 – 12.2015</td></tr>
<tr><td>Parameter [unit]</td><td>Achieved performance</td><td>Requirement</td><td>TR</td><td>Comments</td></tr>
<tr><td>Single measurement precision (1-sigma) in [ppb]</td><td>11.9</td><td>< 34 (T)
< 17 (B)
< 9 (G)</td><td>-</td><td>-</td></tr>
<tr><td>Mean bias [ppb]</td><td>-1.3</td><td>-</td><td>-</td><td>No requirement but value close to zero expected for a high quality data product.</td></tr>
<tr><td>Accuracy: relative systematic error [ppb]</td><td>5.2</td><td>< 10</td><td>Probability that accuracy TR is met: 100%</td><td>-</td></tr>
<tr><td>Stability: Linear bias trend [ppb/year]</td><td>NC</td><td>< 3</td><td>NC</td><td rowspan="2">Time series of available aircraft/AirCore obs are not long enough to compute these 2 parameters</td></tr>
<tr><td>Stability: Year-to-year bias variability [ppb/year]</td><td>NC</td><td>< 3</td><td>-</td></tr>
</table>

Table 22 - Product Quality Summary Table for products CO2_AIRS_NLIS.

<table>
<tr><td colspan="5">Product Quality Summary Table for Product: CO2_AIRS_NLIS
Level: 2, Version: 7.0, Time period covered: 4.2009 – 12.2015</td></tr>
<tr><td>Parameter [unit]</td><td>Achieved performance</td><td>Requirement</td><td>TR</td><td>Comments</td></tr>
<tr><td>Single measurement precision (1-sigma) in [ppb]</td><td>1.32</td><td>< 8 (T)
< 3 (B)
< 1 (G)</td><td>-</td><td>-</td></tr>
<tr><td>Mean bias [ppb]</td><td>-0.43</td><td>-</td><td>-</td><td>No requirement but value close to zero expected for a high quality data product.</td></tr>
</table>

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 already been used for many applications related to the natural and anthropogenic sources and sinks of atmospheric carbon dioxide and methane. Please see the publication list as given on the GHG-CCI website http://www.esa-ghg-cci.org/?q=node/85 (where also links to nearly all publications are given) and see also the references as given in Section REFERENCES.

Nevertheless, we here present some new results obtained using the new C3S products XCO2_OBS4MIPS and XCH4_OBS4MIPS.

Figure 39 shows results of a CO_2 trend analysis based on the XCO2_OBS4MIPS product during 2003-2016. As can be seen, XCO_2 is increasing is approx. 2.1 ppm/year. The derived trend is slightly different for the different latitude bands but the differences are not significant as indicated by the listed uncertainty estimates.

This increase appears to be consistent with CO_2 growth rates as obtained by NOAA at Mauna Loa (obtained from https://www.esrl.noaa.gov/gmd/ccgg/trends/gr.html), which are in the range 1.54 – 3.03 ppm (depending on year) during 2003-2016 (the estimated uncertainty in the Mauna Loa annual mean growth rate is 0.11 ppm/year). The mean NOAA-derived trend is 2 ppm/year during 2000-2010 and 2.2 ppm/year during 2003-2016 (2011-2016: 2.5 ppm/year). The obtained mean growth rate for 2003-2016 of 2.1 ppm/year is in good agreement with the NOAA value of 2.2 ppm/year during the same time period but note that a local CO_2 observation in the troposphere cannot be directly compared with XCO_2, which is a column-averaged quantity. Due to the increase of the mean (NOAA) growth rate with time one would expect that the XCO_2 growth rate is a bit smaller than a growth rate obtained in the lower atmosphere (as vertical mixing requires time).

Note that this first analysis is not very sophisticated and that a more detailed analysis is presented in *Schneising et al., 2014a*, based on an earlier version of the SCIAMACHY XCO_2 product. In that publication growth rates are derived and discussed for individual years.

The XCO2_OBS4MIPS product has also been used to analyse the XCO_2 seasonal cycle amplitude trend. This is motivated by the study of *Wenzel et al., 2016*, who used NOAA observations at Point Barrow, Alaska (and one other site) in the context of “emerging constraints” of climate models. Using more than 30 years of NOAA data at Barrow (located at 71°N) they found an amplitude increase of 0.1 ppm/year. We also performed this analysis and obtained 0.09 +/- 0.05 ppm/year as shown in Figure 40. This is in good agreement with the value reported in *Wenzel et al., 2016.*

We then applied the same analysis to the new XCO2_OBS4MIPS product in the latitude range 50°-70°N as shown in Figure 41 and obtained 0.07 +/- 0.25 ppm/year (note that the uncertainty range is the 3-sigma error of the linear fit). This is in good agreement with the NOAA Barrow data. However, the satellite time series is much shorter than the NOAA time series and the uncertainty of the satellite derived seasonal cycle amplitude trend is so large that the increase is not significant. This indicates that such an application is too demanding for the quite short satellite time series.

Note that the satellite time series shown in Figure 41 has gaps due to the low number of observations at high latitudes in winter. We therefore also performed the same analysis for the latitude band 30°-50°N. The results are shown in Figure 42. Here the time series has no gaps (except for January 2015, where no GOSAT data are available due to issues with the GOSAT satellite) but the trend is still not significant.

Figure 39 – CO_2 trend analysis during 2003-2016 using product XCO2_OBS4MIPS. Top: XCO2_OBS4MIPS time series (thin lines) for three latitude bands (red, green, blue). The latitude ranges and their corresponding trends (including 3-sigma uncertainty range as obtained from the linear fit) are listed in the top left of the figure. The straight (thick) trend lines have been determined by a linear fit. Bottom: XCO_2 time series minus linear trend, i.e., the fit residuum (or seasonal cycle).

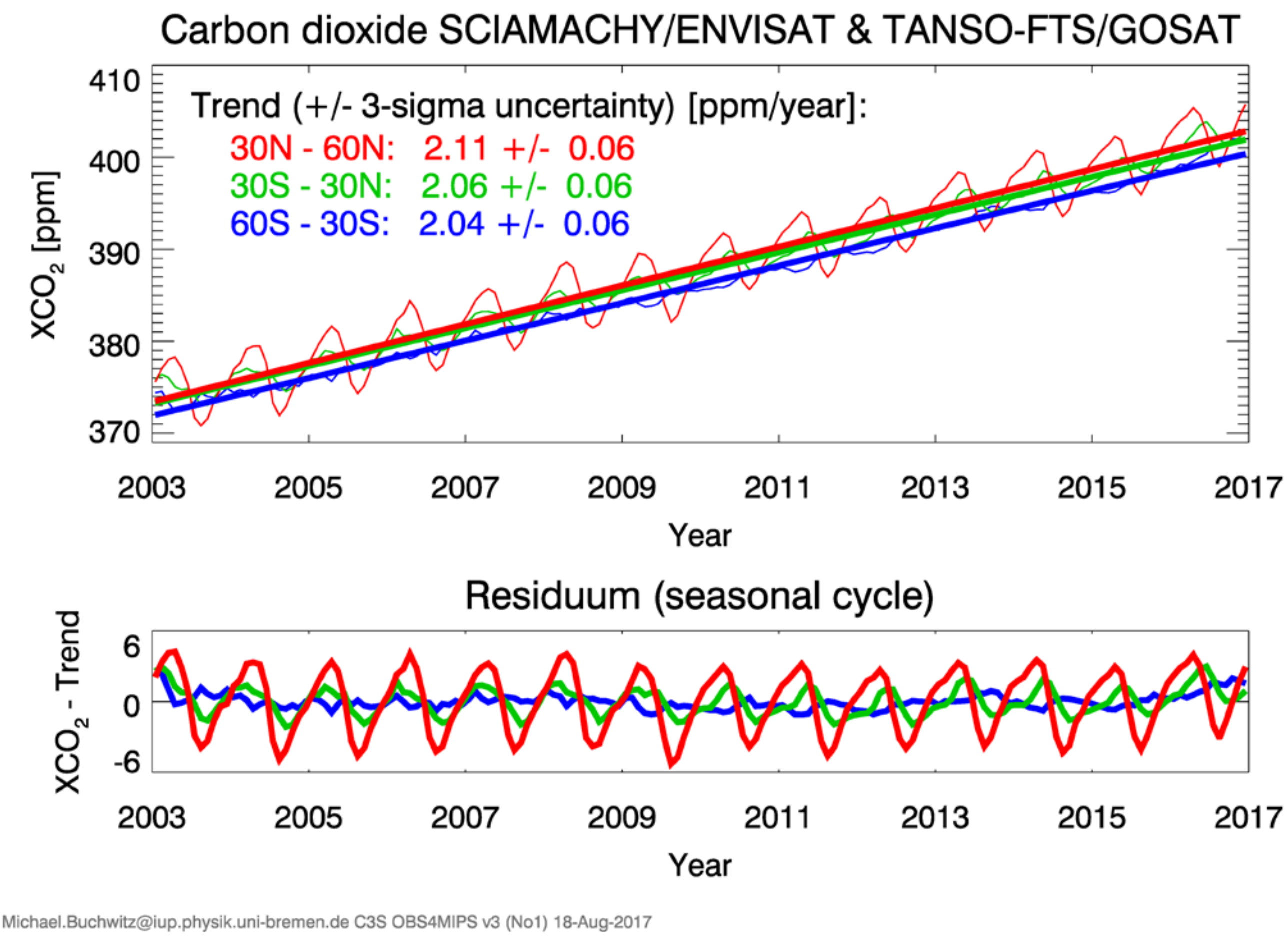


Figure 40 – Analysis of the CO_2 seasonal cycle using NOAA flask measurements from Point Barrow, Alaska. Top: Original CO_2 time series (black line) and corresponding annually averaged time series (red line). Middle: De-trended time series (black line), its maxima (red symbols), its minima (blue symbols) and a (green) line showing for each maximum the corresponding minimum. Bottom: The symbols show the seasonal cycle amplitude as computed from the difference of the maxima and corresponding minima as shown in the middle panel. The red line shows the linear fit and the corresponding slope and its 3-sigma uncertainty are shown in the top of the (bottom) figure.

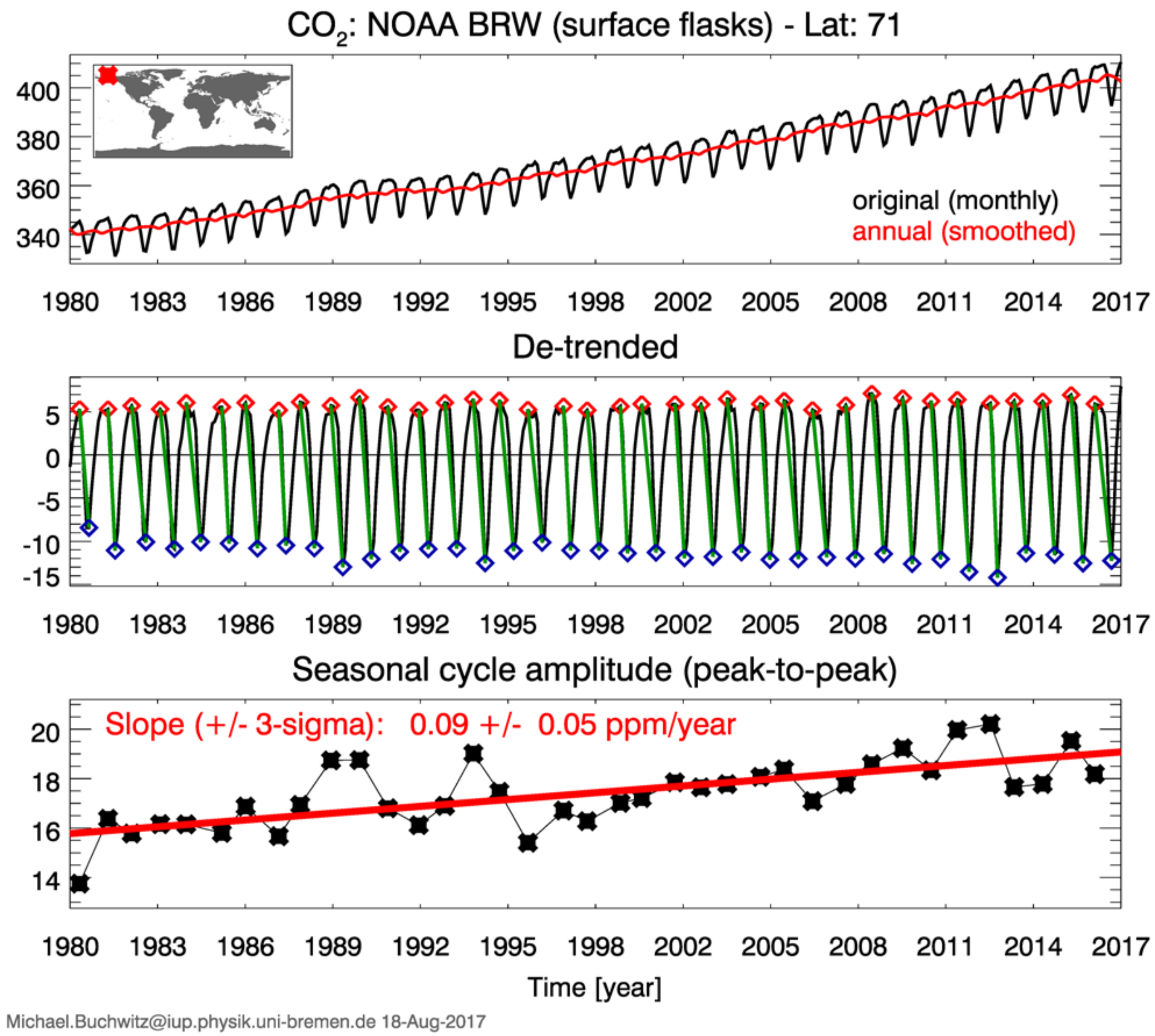


Figure 41 – As Figure 40 but for C3S product XCO2_OBS4MIPS in the latitude band 50°-70°N.

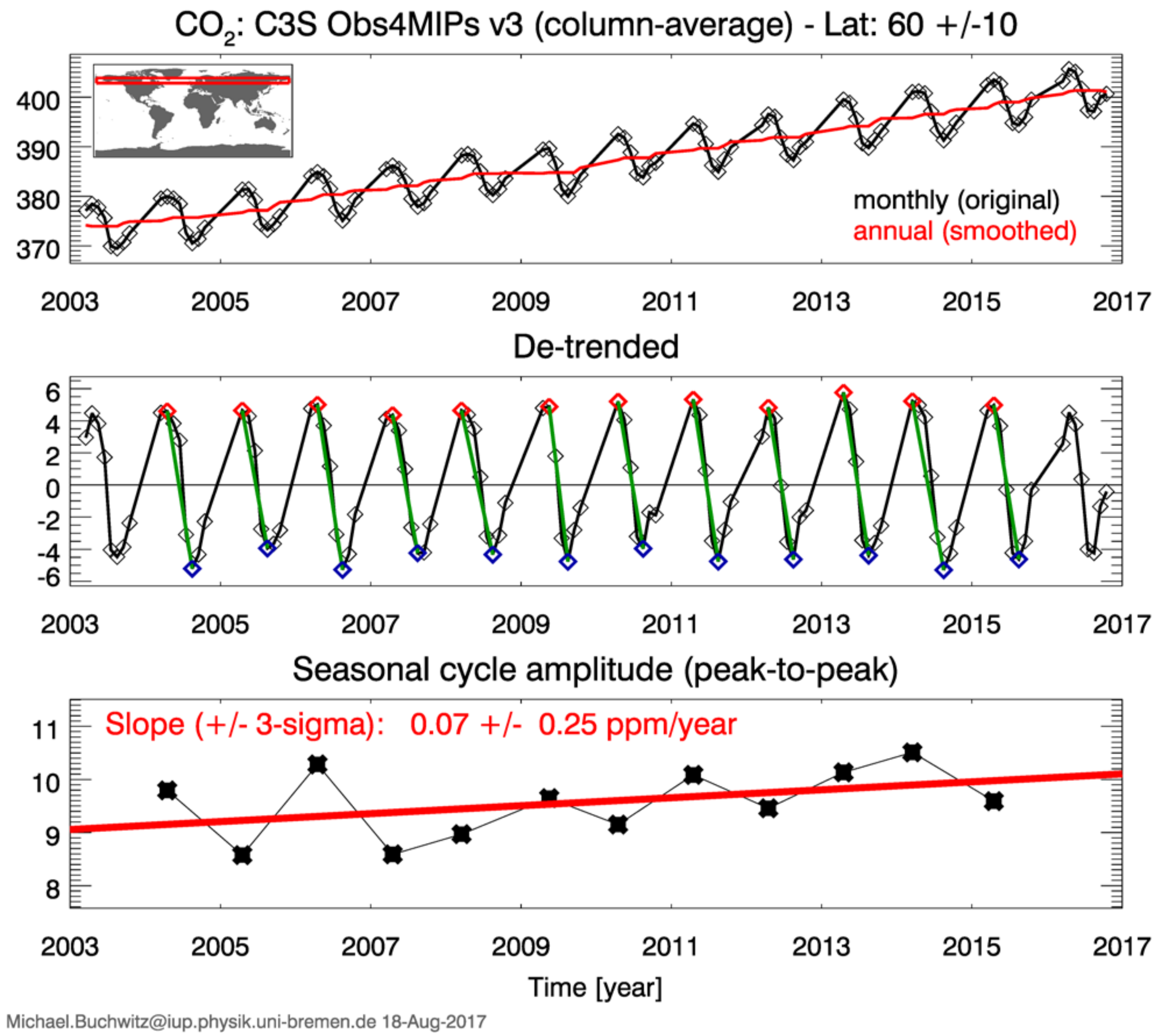
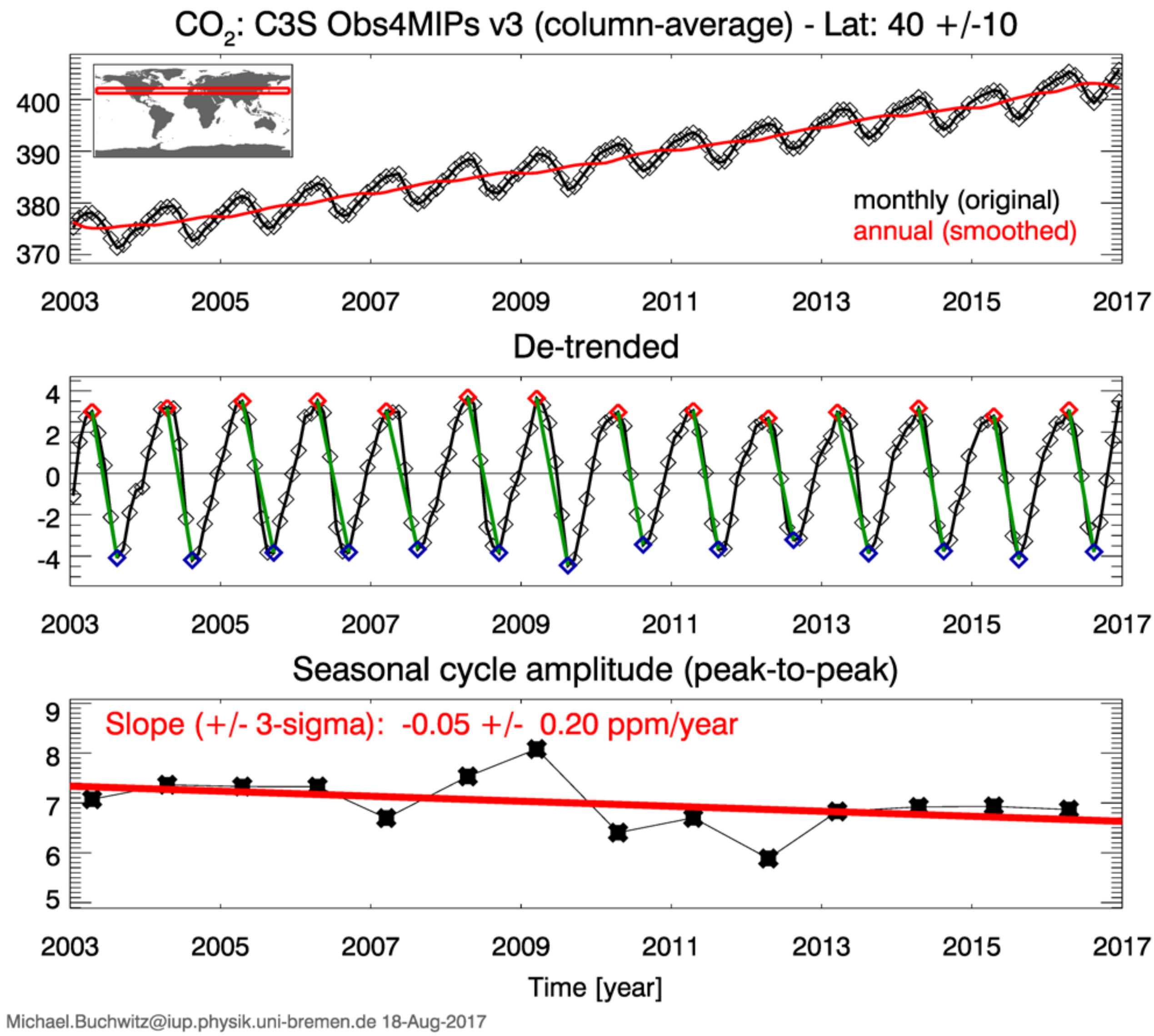
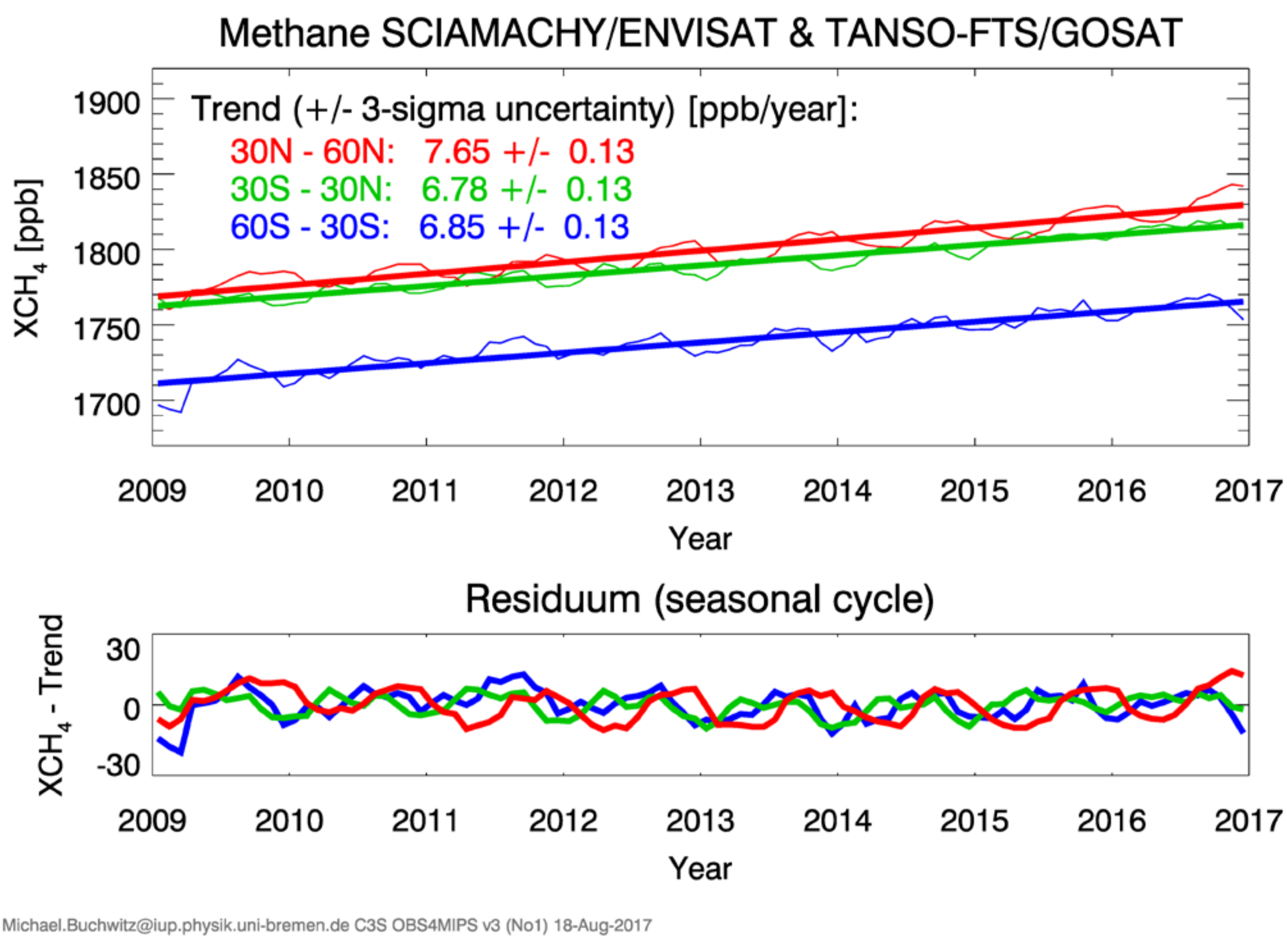


Figure 42 – As Figure 41 but for the latitude band 30°-50°N.



Finally, we also analysed the methane growth rate during recent years using the new XCH4_OBS4MIPS product. The results are shown in Figure 43. The derived increase is approx. 7.6 ppb/year for northern mid-latitudes and slightly less in the tropics and southern hemisphere extra-tropics (around 6.8 ppb/year). This is in reasonable agreement with earlier studies (e.g., Schneising et al., 2011, and references given therein). Simply averaging the annual increases in atmospheric CH_4 based on globally averaged marine surface data from NOAA during 2003-2016 (obtained from https://www.esrl.noaa.gov/gmd/ccgg/trends_ch4/) gives 5.2 ppb/year, which is lower than our estimate. But as for XCO_2 discussed earlier these number can strictly speaking not be compared directly. Nevertheless, it cannot be ruled out that our estimate is a bit too high. Further study is need to investigate this in more detail.

Figure 43 – As Figure 39 but using product XCH4_OBS4MIPS during 2009-2016.



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, accuracy (in terms of spatial / spatio-temporal biases or “relative accuracy” or “relative bias”, i.e., neglecting a possible constant bias or global offset, as obtained from comparison with TCCON XCO_2).

As can be seen, the achieved 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 of better than 3 ppm.

The systematic error requirement is better than 0.5 ppm. The achieved performance is around 0.5 ppm (+/- a few 0.1 ppm). The probability that this requirement has been met is 9% for product CO2_SCI_WFMD and 51% for product CO2_GOS_OCFP and in between these extreme values for the other products. Stability is very good, i.e., close to 100% for all products.

XCH_4:

Figure 2 shows a summary of the achieved performance in terms of single measurement precision, accuracy (in terms of spatial / spatio-temporal biases or “relative accuracy” or “relative bias”, i.e., neglecting a possible constant bias or global offset, as obtained from comparison with TCCON XCO_2).

The required single measurement random error (or precision) is better than 34 ppb (threshold) / better than 17 ppb (breakthrough). The breakthrough requirement is met for the GOSAT products and the threshold requirement is met for the EMMA product. The SCIAMACHY products do not meet the threshold requirement (due to large degradation-related noise after October 2005).

The systematic error (or “relative bias”) requirement of better than 10 ppb (threshold) is met by all GOSAT product and the EMMA product. The SCIAMACHY product accuracy is about 10 ppb. The probability that this requirement is met is nearly 100% for all products except for the SCIAMACHY products where the probability is in the range 38-55%. The stability I very high as the probability that the corresponding requirement (drift < 3 ppb/year) is higher than 90% for all products.

Note however that the SCIAMACHY XCH_4 products suffers from detector degradation in particular after October 2005 resulting in increased scatter and likely also larger systematic error. This affects the following products:

- CH4_SCI_WFMD
- CH4_SCI_IMAP
- XCH4_EMMA (in the time period October 2005 – March 2010; from April 2010 onwards this product is only based on GOSAT data).

5.2 Level 3 XCO_2 and XCH_4 products

The quality assessment results for the XCO_2 product XCO2_OBS4MIPS are:

The estimated accuracy is 0.3 ppm and the probability that the 0.5 ppm requirement is met is 76%.

The linear bias trend is -0.02 +/- 0.04 ppm/year and the probability that the 0.5 ppm/year requirement is met is 99%.

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

The quality assessment results for the XCH_4 product XCH4_OBS4MIPS are:

The estimated accuracy is 2.7 ppb and the probability that the 10 ppb requirement is met is 100%.

The linear bias trend is -0.6 +/- 0.7 ppb/year and the probability that the 3 ppmb/year requirement is met is 97%.

Overall, this product has therefore good accuracy and stability.

Note however that the SCIAMACHY XCH_4 products suffers from detector degradation in particular after October 2005 resulting in increased scatter and likely also larger systematic error. This also affects the XCH4_OBS4MIPS product especially in the time period October 2005 – March 2010 (from April 2010 onwards this product is only based on GOSAT data).

5.3 Level 2 mid-tropospheric products

Product CO2_IASA_NLIS (from IASI on Metop-A) 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 overall bias is estimated to 0.57 ppm). The product is also very stable (-0.01 +/- 0.01 ppm/year (1-sigma)) meeting the requirement for long-term drift.

For product CO2_IASB_NLIS (from IASI on Metop-B) the performance seems to be similar apart from an offset to product CO2_IASA_NLIS of 2 ppm (low bias of Metop-B product).

Product CH4_IASA_NLIS (from IASI on Metop-A) appears to meet the “relative systematic error” requirement of better than 10 ppb: the estimated relative accuracy is about 5.2 ppb (the overall bias is estimated to -1.3 ppb). The product appears to be quite stable but a quantitative assessment could not be carried out due to lack of reference data. For product CH4_IASB_NLIS (from IASI on Metop-B) the performance seems to be similar.

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

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6. Acknowledgement

We acknowledge previous funding by the European Space Agency (ESA) via Climate Change Initiative (CCI) project GHG-CCI. This funding significantly enhanced the quality of the retrieval algorithms and related documentation. This resulted in more mature data products as needed for an operational project such as the Copernicus Climate Change Service (C3S). We also acknowledge the availability of GOSAT data products via the ESA GOSAT Third Party Mission (TPM) archive.

We are also very grateful to the GOSAT team in Japan comprising the Japan Aerospace Exploration Agency (JAXA), the National Institute for Environmental Studies (NIES), and the Ministry of the Environment (MOE) for providing access to the GOSAT Level 1 and Level 2 data products via the GOSAT Data Archive Service (GDAS) hosted by NIES.

7. List of ANNEXes

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 products XCO2_EMMA, XCH4_EMMA

Describes the validation of the multi-sensor merged XCO_2 and XCH_4 Level 2 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 are available from:

https://climate.copernicus.eu/

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