ECMWF COPERNICUS REPORT

Copernicus Climate Change Service

Product User Guide and Specification (PUGS) – Main document for Greenhouse Gas (GHG: CO_2 & CH_4) data set CDR6 (01.2003-12.2021)

C3S2_312a_Lot2_DLR – Atmosphere

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History of modifications

Version	Date	Description of modification	Chapters / Sections
1.3	20-October-2017	New document for data set CDR1 (temporal coverage: 2003-2016)	All
2.0	16-October-2018	Update for data set CDR2 (temporal coverage: 2003-2017)	All
3.0	12-August-2019	Update for data set CDR3 (temporal coverage: 2003-2018)	All
4.0	17-September-2020	Update for data set CDR4 (temporal coverage: 2003-mid2019)	All
5.0	18-February-2021	Update for data set CDR5 (temporal coverage: 2003-mid2020)	All
6.0	4-August-2022	Update for data set CDR6 (temporal coverage: 2003-2021)	All
6.1	6-December-2022	Update after review (use of new template, several improvements at various places)	All
6.2	14-February-2023	Update after 2nd review with several improvements at various places.	All
6.3	18-April-2023	Update after 3rd review with several improvements at various places.	All

List of datasets covered by this document

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

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

Related documents

Reference ID	Document
D1	**GCOS-154:** Global Climate Observing System (GCOS), SYSTEMATIC OBSERVATION REQUIREMENTS FOR SATELLITE-BASED 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, 2011. Link: https://library.wmo.int/doc_num.php?explnum_id=3710
D2	**GCOS-195:** Status of the Global Observing System for Climate, GCOS-195, 2015. Link: https://library.wmo.int/doc_num.php?explnum_id=7213
D3	**GCOS-200:** The Global Observing System for Climate: Implementation Needs, GCOS 2016 Implementation Plan, World Meteorological Organization (WMO), GCOS-200 (GOOS-214), pp. 325, 2016. Link: https://unfccc.int/sites/default/files/gcos_ip_10oct2016.pdf
D4	**ESA-CCI-GHG-URDv3.0:** Chevallier, F., et al., User Requirements Document (URD), ESA Climate Change Initiative (CCI) GHG-CCI project, Version 3.0, 17 Feb 2020, pp. 42, 2020. Link: https://www.iup.uni-bremen.de/carbon_ghg/docs/GHG-CCIplus/URD/URDv3.0_GHG-CCIp_Final.pdf
D5	**CMUG-RBD, 2012:** Climate Modelling User Group Requirements Baseline Document, Deliverable 1.2, Number D1.2, ESA Climate Change Initiative (CCI), Version 1.6, 17 Dec 2012, 2012. Link: https://climate.esa.int/media/documents/CMUG_D1.2_URD_v2.0.pdf
D6	**GCOS-245:** The 2022 GCOS ECVs Requirements, WMO, pp. 244, 2022. Link: https://library.wmo.int/doc_num.php?explnum_id=11318
D7	**TRD GAD GHG, 2021:** Buchwitz, M., Reuter, M., Schneising-Weigel, O., Aben, I., Wu, L., Hasekamp, O. P., Boesch, H., Di Noia, A., Crevoisier, C., Armante, R.: Target Requirement and Gap Analysis Document, Copernicus Climate Change Service (C3S) project on satellite-derived Essential Climate Variable (ECV) Greenhouse Gases (CO_2 and CH_4) data products, Version 3.1, 19-February-2021, pp. 81, 2021. Latest version: http://wdc.dlr.de/C3S_312b_Lot2/Documentation/GHG/C3S2_312a_Lot2_TRD-GAD_GHG_latest.pdf

D8	**ATBD GHG, 2023:** Buchwitz, M., Barr, A., Boesch, H., Borsdorff, T., Crevoisier, C., Di Noia, A., Hasekamp, O. P., Landgraf, J., Meilhac, N., Parker, R., Reuter, M., Schneising-Weigel, O.: Algorithm Theoretical Basis Document (ATBD) – Main document for Greenhouse Gas (GHG: CO_2 & CH_4) data set CDR6 (01.2003-12.2021), C3S project C3S2_312a_Lot2_DLR, v6.2, 31/01/2023, pp. 44, 2023. Link: https://www.iup.uni-bremen.de/carbon_ghg/docs/C3S/CDR6_2003-2021/C3S2_312a_Lot2_D-WP1_ATBD-2022-GHG_MAIN_v6.2.pdf
D9	**PQAR GHG, 2023:** Buchwitz, M., Barr, A., Boesch, H., Borsdorff, T., Crevoisier, C., Di Noia, A., Hasekamp, O. P., Landgraf, J., Meilhac, N., Parker, R., Reuter, M., Schneising-Weigel, O.: Product Quality Assessment Report (PQAR) – Main document for Greenhouse Gas (GHG: CO_2 & CH_4) data set CDR6 (01.2003-12.2021), C3S project C3S2_312a_Lot2_DLR, v6.3, 02/03/2023, pp. 88, 2023. Link: https://www.iup.uni-bremen.de/carbon_ghg/docs/C3S/CDR6_2003-2021/C3S2_312a_Lot2_D-WP2_PQAR-2022-GHG_MAIN_v6.3.pdf

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
GOS	GOSAT
GO2	GOSAT-2
GOME	Global Ozone Monitoring Experiment
GMES	Global Monitoring for Environment and Security
GOSAT	Greenhouse Gases Observing Satellite

GOSAT-2	Greenhouse Gases Observing Satellite 2
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-tropospheric CO_2 and CH_4 retrieval algorithm
NOAA	National Oceanic and Atmospheric Administration
Obs4MIPs	Observations for Climate Model Intercomparisons
OCFP	OCO-2 Full Physics (FP) algorithm (used by Univ. Leicester)
OCO	Orbiting Carbon Observatory
OCPR	OCO-2 Proxy (PR) algorithm (used by Univ. Leicester)
OE	Optimal Estimation
PBL	Planetary Boundary Layer
ppb	Parts per billion
ppm	Parts per million
PQAD	Product Quality Assurance Document
PQAR	Product Quality Assessment Report
PR	(light path) PRoxy retrieval method
PVIR	Product Validation and Intercomparison Report
QA	Quality Assurance
QC	Quality Control
RemoTeC	Retrieval algorithm developed by SRON
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
SRFP	SRON's Full Physics (FP) algorithm (also referred to a RemoTeC FP)
SRPR	SRON's Proxy (PR) algorithm (also referred to a RemoTeC PR)
SWIR	Short Wava Infra Red
TANSO	Thermal And Near infrared Sensor for carbon Observation
TANSO-FTS	Fourier Transform Spectrometer on GOSAT
TANSO-FTS-2	Fourier Transform Spectrometer on GOSAT-2
TBC	To be confirmed
TBD	To be defined / to be determined
TCCON	Total Carbon Column Observing Network
TIR	Thermal Infra Red
TR	Target Requirements
TRD	Target Requirements Document
WFM-DOAS (or WFMD)	Weighting Function Modified DOAS
UoL	University of Leicester, United Kingdom
URD	User Requirements Document
WMO	World Meteorological Organization
Y2Y	Year-to-year (bias variability)

General definitions

Essential climate variable (ECV)

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

Climate data record (CDR)

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

Fundamental climate data record (FCDR)

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

Thematic climate data record (TCDR)

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

Intermediate climate data record (ICDR)

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

Satellite data processing levels

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

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

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Scope of document

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

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

These satellite-derived data products are (see also *Reuter et al., 2020*):

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

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

For an overview of the merged Level 2 data products XCO2_EMMA and XCH4_EMMA and of the merged Level 3 data products XCO2_OBS4MIPS and XCH4_OBS4MIPS see also Reuter et al., 2020.

Requirements on data quality are formulated in the corresponding Target Requirement Document (TRD) (Reference ID *D7*). They are based on requirements as formulated in documents *D1*, *D2*, *D3, D4* and *D5*.

The main purpose of this document is to describe the satellite-derived CO_2 and CH_4 greenhouse gas (GHG) ECV data products for users of these data products.

Note that this document does not contain a description of the retrieval algorithms which have been used to generate these products. These algorithms are described in a separate document (Reference ID *D8*): Algorithm Theoretical Basis Document (ATBD).

Note also that this document does not contain detailed validation results. Detailed data quality and validation results are reported in a separate document (Reference ID *D9*): Product Quality Assessment Report (PQAR).

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

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

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

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

Executive summary

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 modelling) to obtain (improved) information on their (primarily surface) sources and sinks.

CO_2 and CH_4, have relatively long atmospheric lifetimes. Because of this, and associated human emissions, the atmospheric concentrations of these gases can be relatively high compared to some other atmospheric trace gases. Moderate to strong (surface) source or sink typically may only result in relatively small local or regional change (enhancement or depletion relative to the surrounding region) in their vertical columns or their mid-tropospheric concentration. Given the small magnitude of these perturbations, it is important to give appropriate consideration to random and systematic errors.

In order to obtain source/sink information from the atmospheric observations it is therefore required to consider atmospheric transport (and associated atmospheric chemistry) as well as the exact time and location of observations.

As a consequence, the most relevant data products are 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 (*D7*) are, therefore, mostly L2 requirements. However, for XCO_2 and XCH_4 also (gridded) Level 3 (L3) products have been generated (in OBS4MIPS format).

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

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

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

The C3S GHG data products are generated from the satellite instruments SCIAMACHY/ENVISAT, TANSO-FTS/GOSAT, TANSO-FTS-2/GOSAT-2 (XCO_2 and XCH_4 products) and AIRS and IASI (mid-tropospheric products). Products from SCIAMACHY and AIRS have been generated in pre-cursor projects and no updates are generated within this project; the corresponding GHG products are available via the Copernicus Climate Data Store (CDS, https://cds.climate.copernicus.eu/). However, SCIAMACHY products are used as input for the generation of the four merged products, which are based on combining individual sensor products. These products are: XCO2_EMMA, XCO2_OBS4MIPS, XCH4_EMMA, and XCH4_OBS4MIPS. For the products XCO2_EMMA and XCO2_OBS4MIPS also Level 2 products from NASA's OCO-2 mission have been used as input products (see also Reuter et al., 2020).

All data products are available as Level 2 (individual ground pixels) products in NetCDF format (NetCDF-4 classic format in-line with Climate and Forecasting (CF) convention 3).

The XCO_2 and XCH_4 Level 2 products are available for individual sensors (GOSAT and GOSAT-2) but also as merged multi-sensor Level 2 (so called EMMA) products (including products from SCIAMACHY/ENVISAT as generated in pre-cursor projects). In addition, also merged Level 3 (i.e., gridded) products in OBS4MIPS format are available for XCO_2 and XCH_4.

This C3S project is essentially the operational continuation of the research and development (R&D) pre-cursor project GHG-CCI of ESA's Climate Change Initiative (CCI).

The first C3S GHG data set - Climate Data Record 1 (CDR1) - covered the period 2003-2016 and had been delivered to ECMWF in 2017. The second data set - Climate Data Record 2 (CDR2) - covered the period 2003-2017 and has been made available for the C3S CDS in 2018. This document is an update of document PUGS for the latest CDR data set CDR6 covering the period 2002-2021.

This document is the MAIN PUGS document. It provides an overview of the products by describing the data format and content which is relevant for all users. However, each product may also contain additional – typically algorithm specific – information, which may be useful for certain applications. Details on each product are provided in separate ANNEXes:

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

1. Overview of data products

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

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

- Column-averaged dry-air mixing ratios (mole fractions) of CO_2 and CH_4, denoted XCO_2 (in parts per million, ppm, see Figure 1) and XCH_4 (in parts per billion, ppb, see Figure 2).
- Mid-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 including the definition of key requirements (e.g., GCOS-154, GCOS-200). In recent years several satellite-derived ECV data products, including CO_2 and CH_4 (e.g., Buchwitz et al., 2013a, 2016, 2017), have been generated in particular in the framework of the Climate Change Initiative (CCI) of ESA (e.g., Hollmann et al., 2013).

Previous versions 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; Gier et al., 2020) and other models (e.g., Schneising et al., 2014a; Parker et al., 2016)

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

Figure 1 - Overview of the C3S XCO_2 product 2003-2021 in terms of global maps and time series.

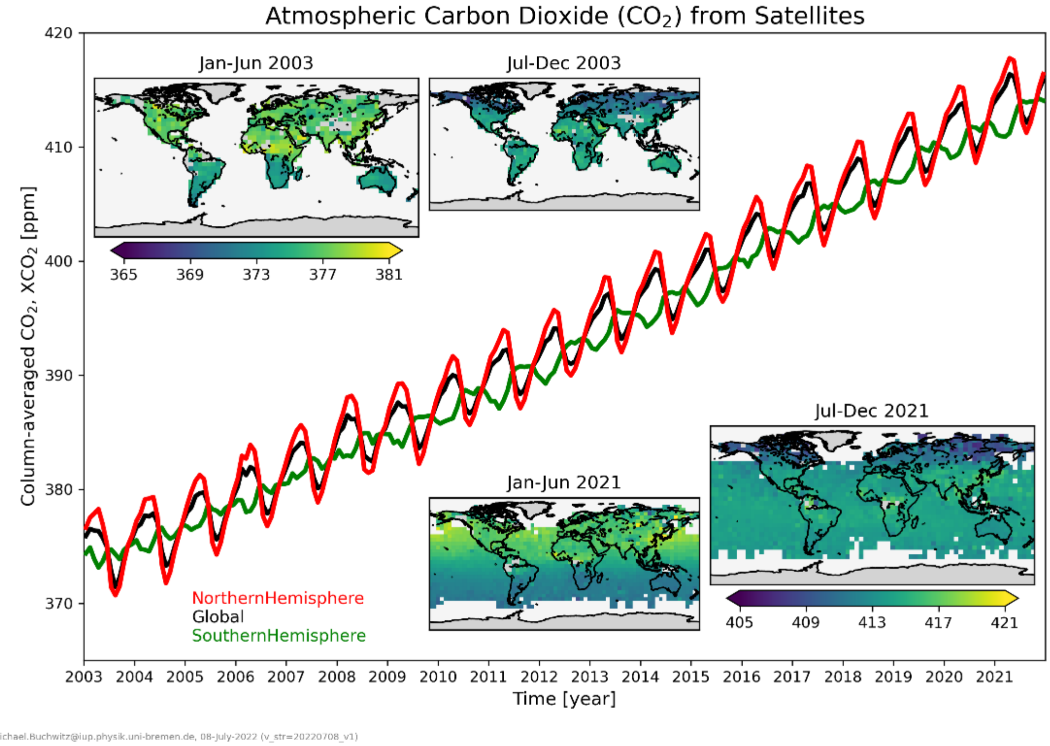
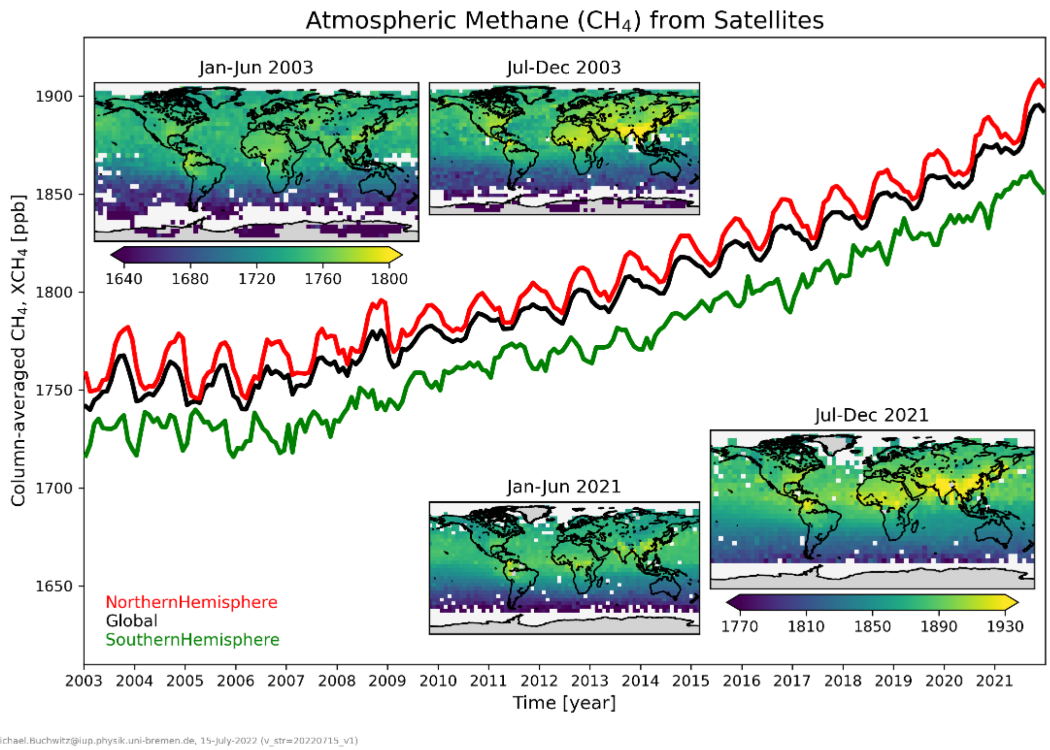


Figure 2 - Overview of the C3S XCH_4 product during 2003-2021 in terms of global maps and time series.



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 (down looking) 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 retrieve "total column information" but do not permit to retrieve (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).

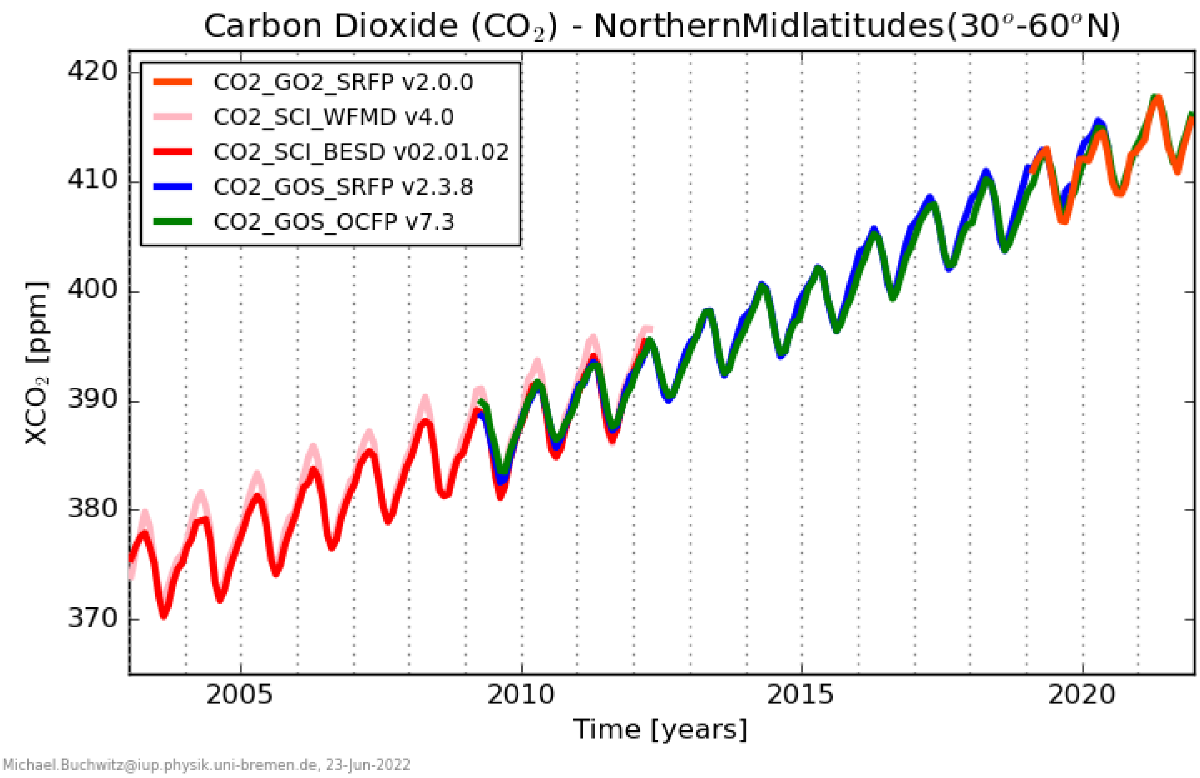
1.1.2 XCO_2

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; Noël et al., 2021, 2022; Reuter et al., 2011; 2013; Schneising et al., 2011; Yoshida et al., 2013). These products have been validated using Total Carbon Column Observing Network (TCCON) (Wunch et al., 2010, 2011, 2015) XCO_2 ground based observations (e.g., Dils et al., 2014). In this document, the latest versions of these data products are described.

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

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



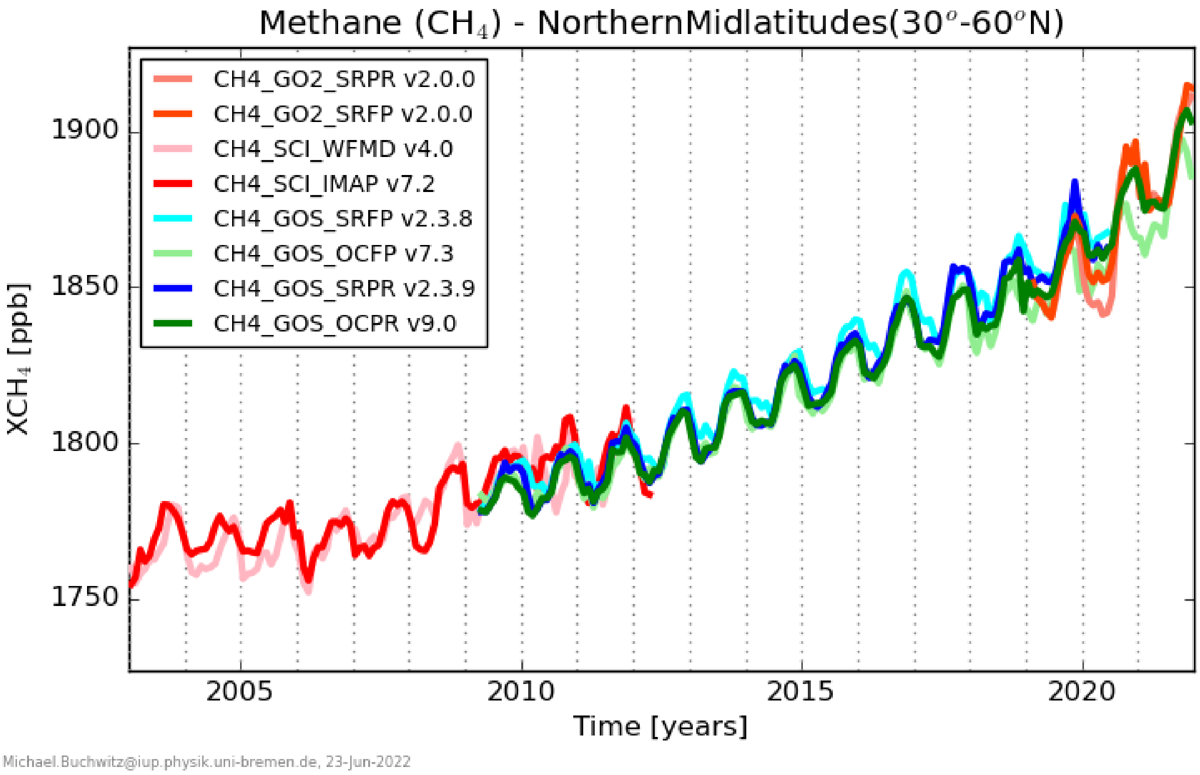
1.1.3 XCH_4

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; Noël et al., 2022; 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, the latest versions of these data products are described.

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

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



1.1.4 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, products are generated using «Full Physics» (FP) and «Proxy» (PR) retrieval algorithms. For a discussion of FP versus PR algorithms see, for example, Schepers et al., 2012. Each type of algorithm has different advantages and disadvantages. Typically, the PR products contain much more data as quality filtering can be less strict but the PR algorithms use 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 3 - Overview XCO_2 data products. In column "(Planned) Availability" the first data is the (planned) delivery date and the period with the start and end time is the period covered by the data product. Also listed are dates and period of previous deliveries. The latest entry corresponds to the latest data product version and covers the longest data product period. CDR 5 refers to the previously generated "Climate Data Record" data set and CDR 6 refer to the new data set described in this document. Column "Availability" lists the (planned) date of availability of the data products in the Copernicus Climate Data Store[1] followed by the period covered by the corresponding product.

Product ID	Level	Sensor(s)	CDR: (Planned) Availability: Temporal coverage	Comments
CO2_GOS_OCFP	2	GOSAT	CDR 5: Jul. 2021: 2009-mid 2020 CDR 6: Dec. 2022: 2009-2021	Univ. Leicester's "Full Physics" (FP) algorithm
CO2_GO2_SRFP	2	GOSAT-2	CDR 6: Dec. 2022: 2019-2021	SRON's "Full Physics" (FP) algorithm
XCO2_EMMA	2	Merged SCIAMACHY, GOSAT, OCO-2	CDR 5: Jul. 2021: 2003-mid 2020 CDR 6: Dec. 2022: 2003-2021	Univ. Bremen's Level 2 merging algorithm
XCO2_OBS4MIPS	3	Merged SCIAMACHY, GOSAT, OCO-2	CDR 5: Jul. 2021: 2003-mid 2020 CDR 6: Dec. 2022: 2003-2021	Gridded EMMA product in Obs4MIPs format

[1] https://cds.climate.copernicus.eu (last access: 3-Apr-2023)

Table 4 - Overview XCH_4 data products. In column “(Planned) Availability” the first data is the (planned) delivery date and the period with the start and end time is the period covered by the data product . Also listed are dates and period of previous deliveries. The latest entry corresponds to the latest data product version and covers the longest data product period. CDR 5 refers to the previously generated “Climate Data Record” data set and CDR 6 refer to the new data set described in this document. Column “Availability” lists the (planned) date of availability of the data products in the Copernicus Climate Data Store followed by the period covered by the corresponding product.

Product ID	Level	Sensor(s)	CDR: (Planned) Availability: Temporal coverage	Comments
CH4_GOS_OCPR	2	GOSAT	CDR 5: Jul. 2021: 2009-mid 2020 CDR 6: Dec. 2022: 2009-2021	Univ. Leicester’s “Proxy” (PR) algorithm
CH4_GOS_OCFP	2	GOSAT	CDR 5: Jul. 2021: 2009-mid 2020 CDR 6: Dec. 2022: 2009-2021	Univ. Leicester’s “Full Physics” (FP) algorithm
CH4_GO2_SRPR	2	GOSAT-2	CDR 6: Dec. 2022: 2019-2021	SRON’s “Proxy” (PR) algorithm
CH4_GO2_SRFP	2	GOSAT-2	CDR 6: Dec. 2022: 2019-2021	SRON’s “Full Physics” (FP) algorithm
XCH4_EMMA	2	Merged SCIAMACHY & GOSAT	CDR 5: Jul. 2021: 2003-mid 2020 CDR 6: Dec. 2022: 2003-2021	Univ. Bremen’s Level 2 merging algorithm
XCH4_OBS4MIPS	3	Merged SCIAMACHY & GOSAT	CDR 5: Jul. 2021: 2003-mid 2020 CDR 6: Dec. 2022: 2003-2021	Gridded EMMA product in Obs4MIPs format

On the following pages maps of these products are shown so that users can see what a product «looks like».

Figure 5 shows product CO2_GOS_OCFP for January to June 2021 (top) and July to December 2021 (bottom) gridded at 1°x1°. These maps have been computed from the Level 2 product files simply by averaging all individual footprint (ground pixel) XCO_2 data within the specified period with quality flag "good" (i.e., with xco2_quality_flag = 0) as contained within the 1°x1° grid cells (using only the ground pixel centre coordinates).

Figure 6 shows the corresponding maps for product CO2_GO2_SRFP.

Figure 7 shows the corresponding maps for product CH4_GOS_OCFP. This « full physics » (FP) GOSAT product is sparser compared to the corresponding « proxy » (PR) product CH4_GOS_OCPR shown in Figure 8.

The reason why PR products typically contain more data points and better coverage compared to FP products is that PR products suffer less from potential biases and therefore require less strict quality filtering resulting in more data points with quality flag "good" in the final product files. PR products benefit from cancelling of systematic errors as they are based on computing the ratio of two retrieved quantities with similar systematic errors; here the retrieved vertical column of CH_4 is divided by the retrieved CO_2 vertical column. Therefore, the number of "good" retrievals is typically higher in PR products compared to FP products. However, PR products also have a disadvantage as a CO_2 model is needed and used to correct for the CO_2 dependence as introduced by computing the ratio with the retried CO_2 column. For more information on this topic please see Schepers et al., 2012, and references given therein.

Figure 9 shows the corresponding GOSAT-2 maps for product CH4_GO2_SRFP. This FP GOSAT-2 product is sparser compared to the corresponding PR product CH4_GO2_SRPR shown in Figure 10.

Figure 5 - XCO_2 product CO2_GOS_OCFP. Top: January to June 2021. Bottom: July – December 2021.

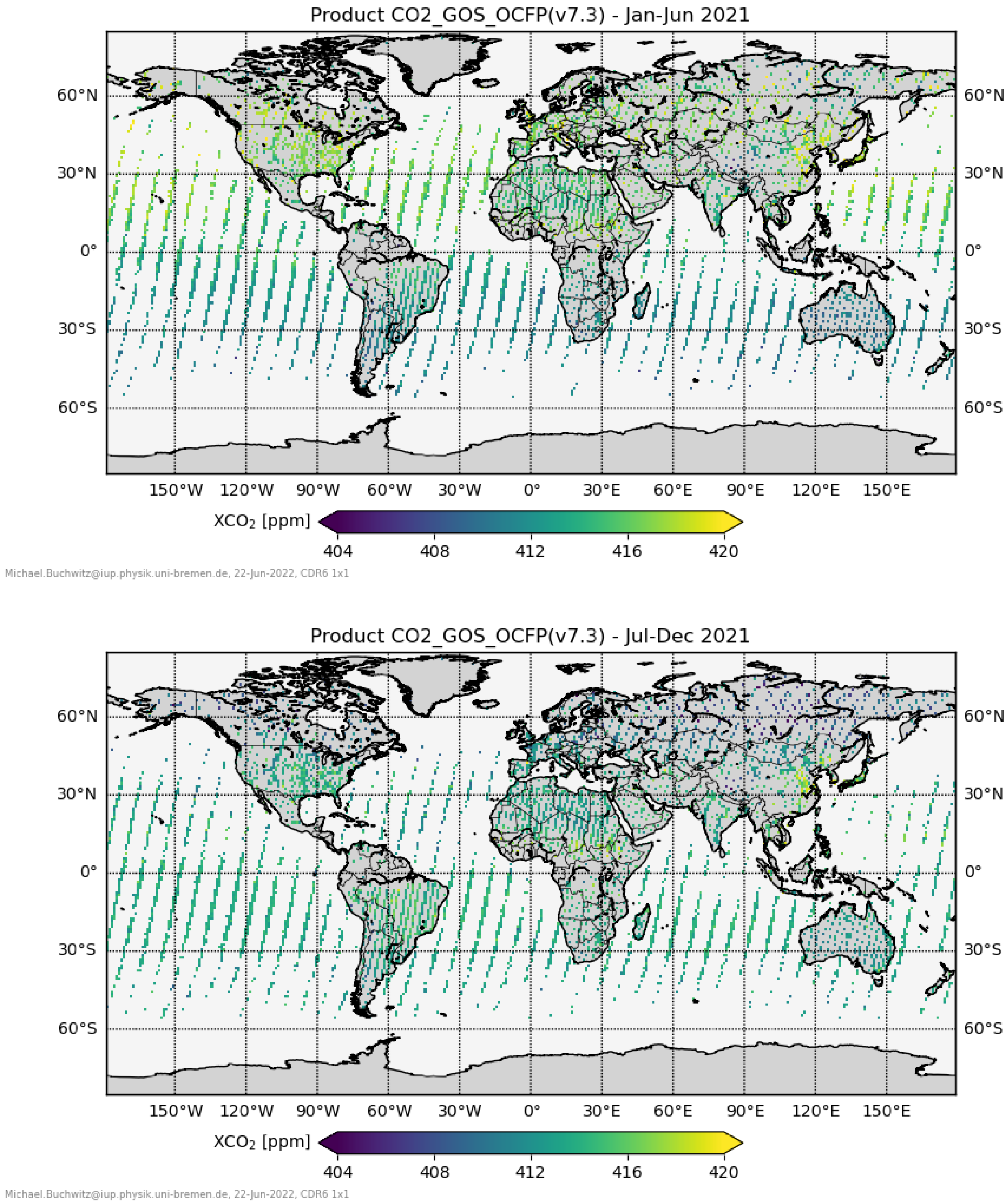
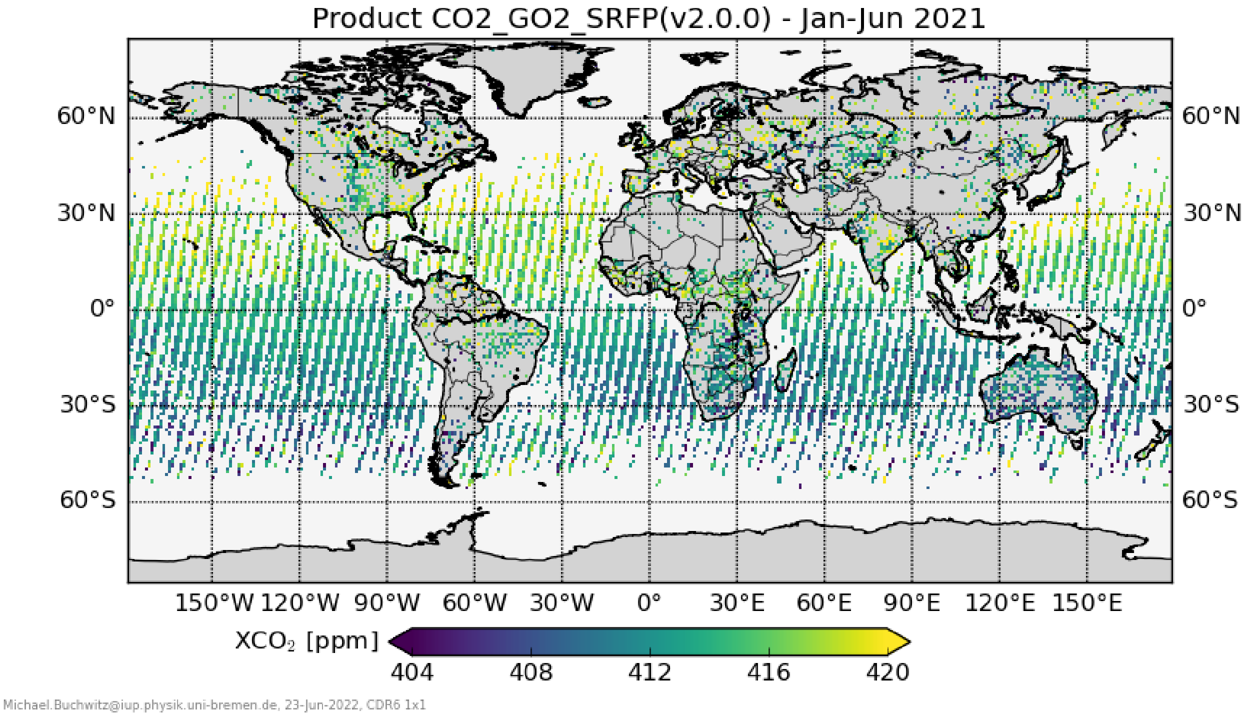


Figure 6 - XCO_2 product CO2_GO2_SRFP. Top: January to June 2021. Bottom: July – December 2021.



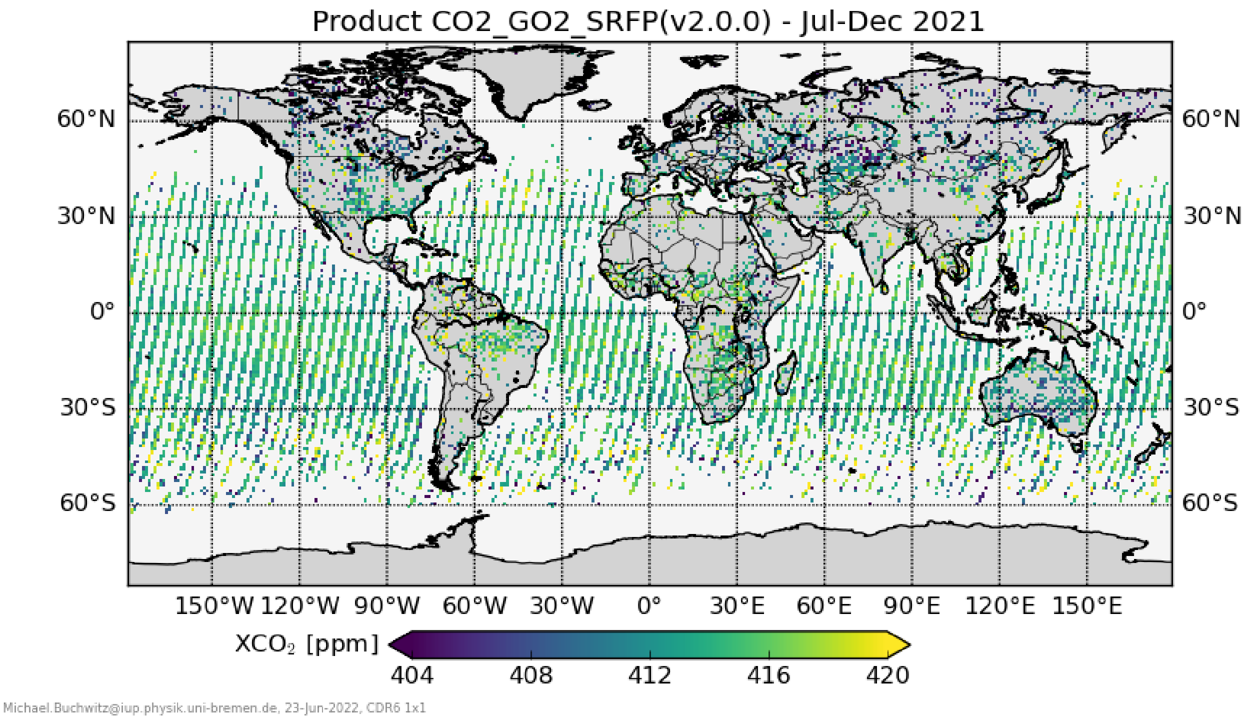
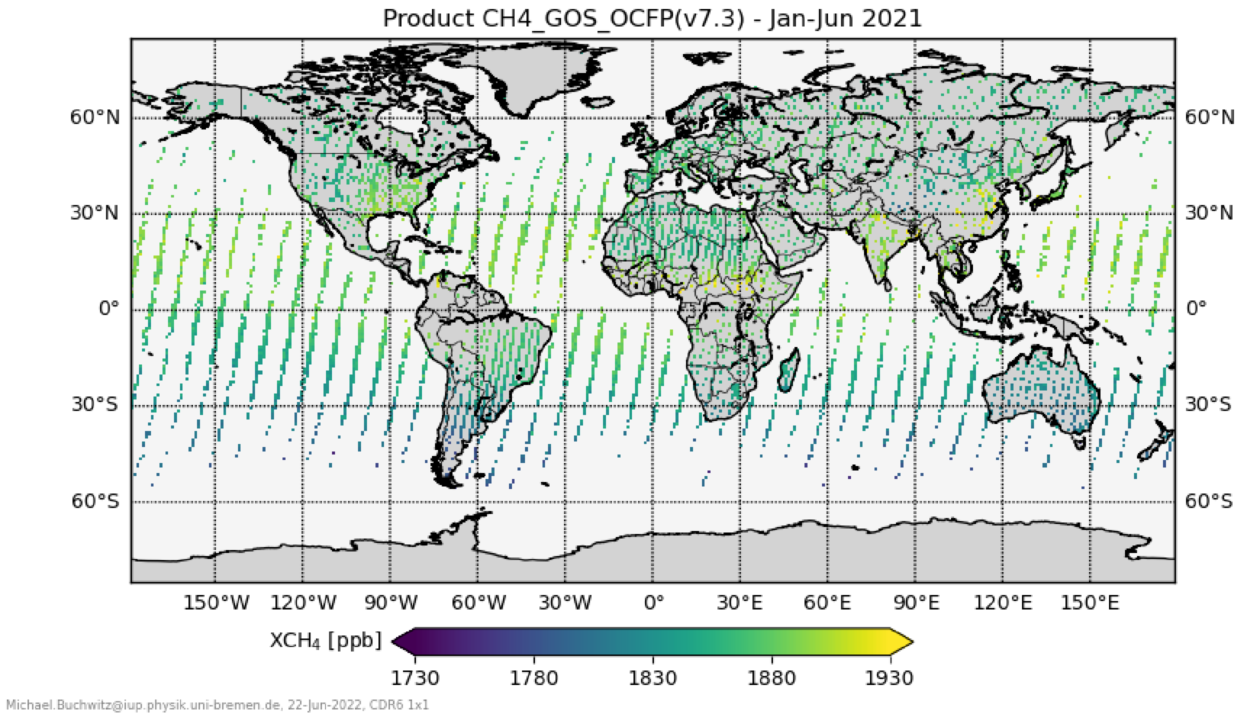


Figure 7 - XCH_4 product CH4_GOS_OCFP. Top: January to June 2021. Bottom: July – December 2019.



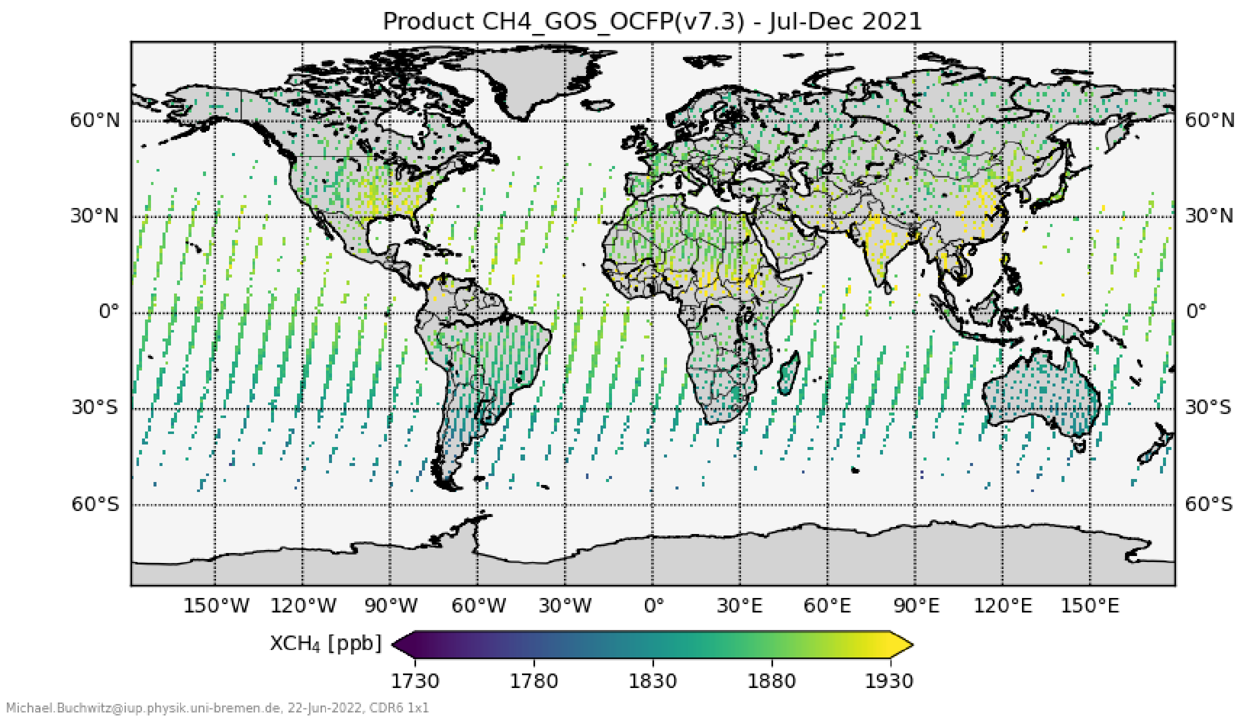
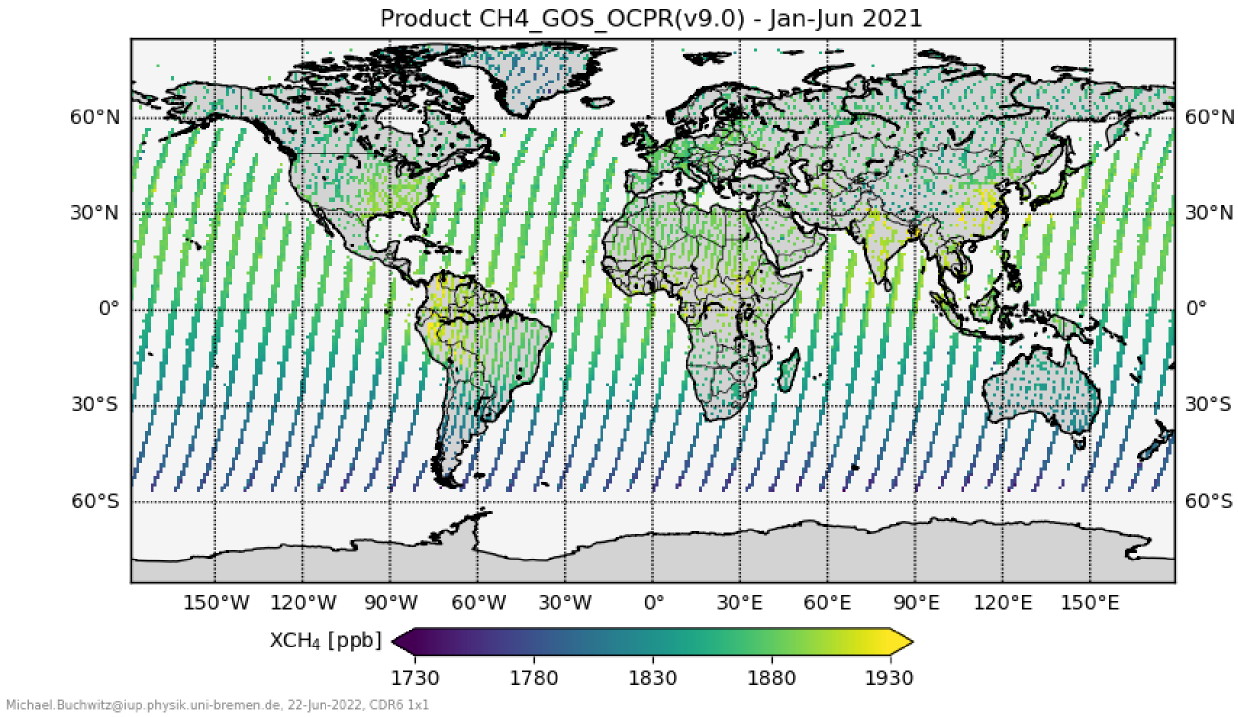


Figure 8 - XCH_4 product CH4_GOS_OCPR. Top: January to June 2021. Bottom: July – December 2021.



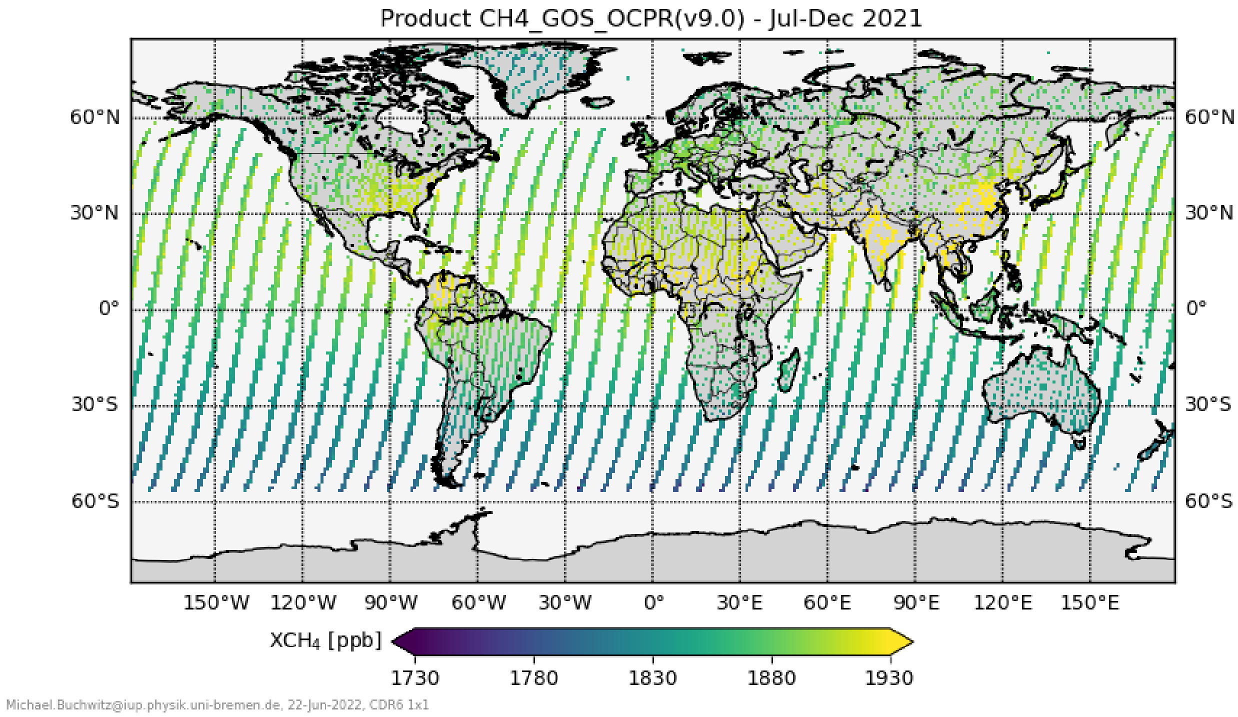
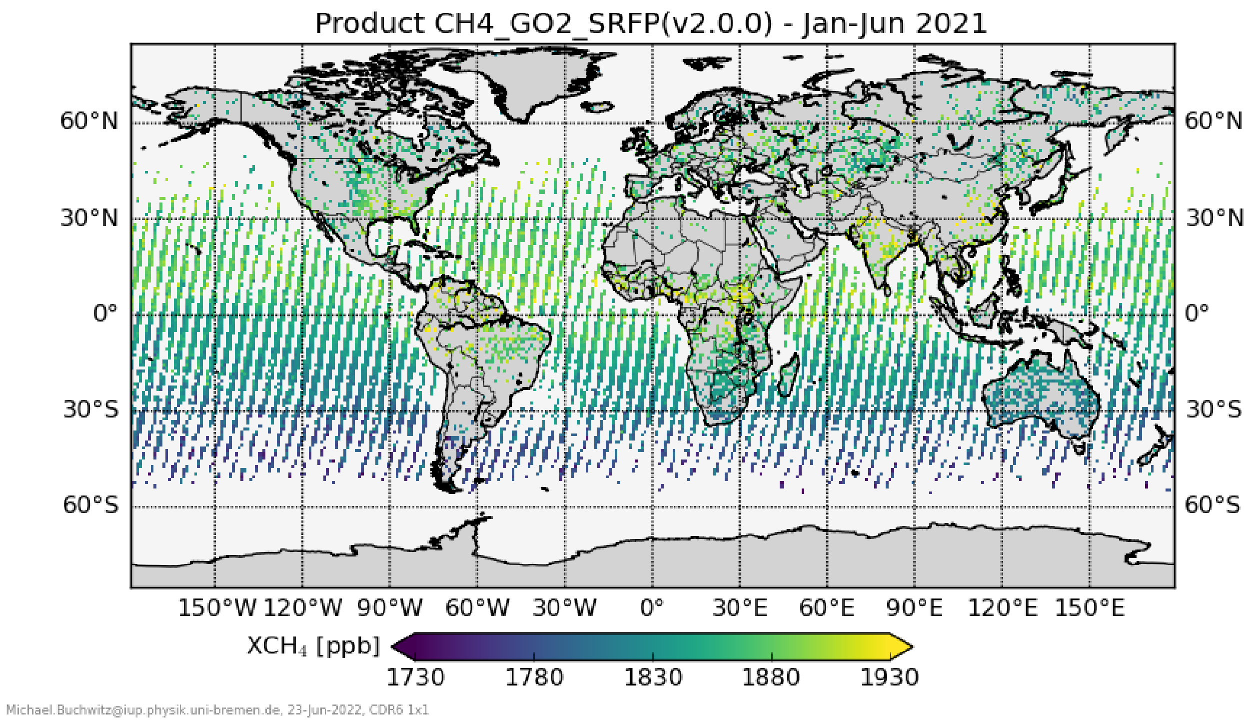


Figure 9 - XCH_4 product CH4_GO2_SRFP. Top: January to June 2021. Bottom: July – December 2021.



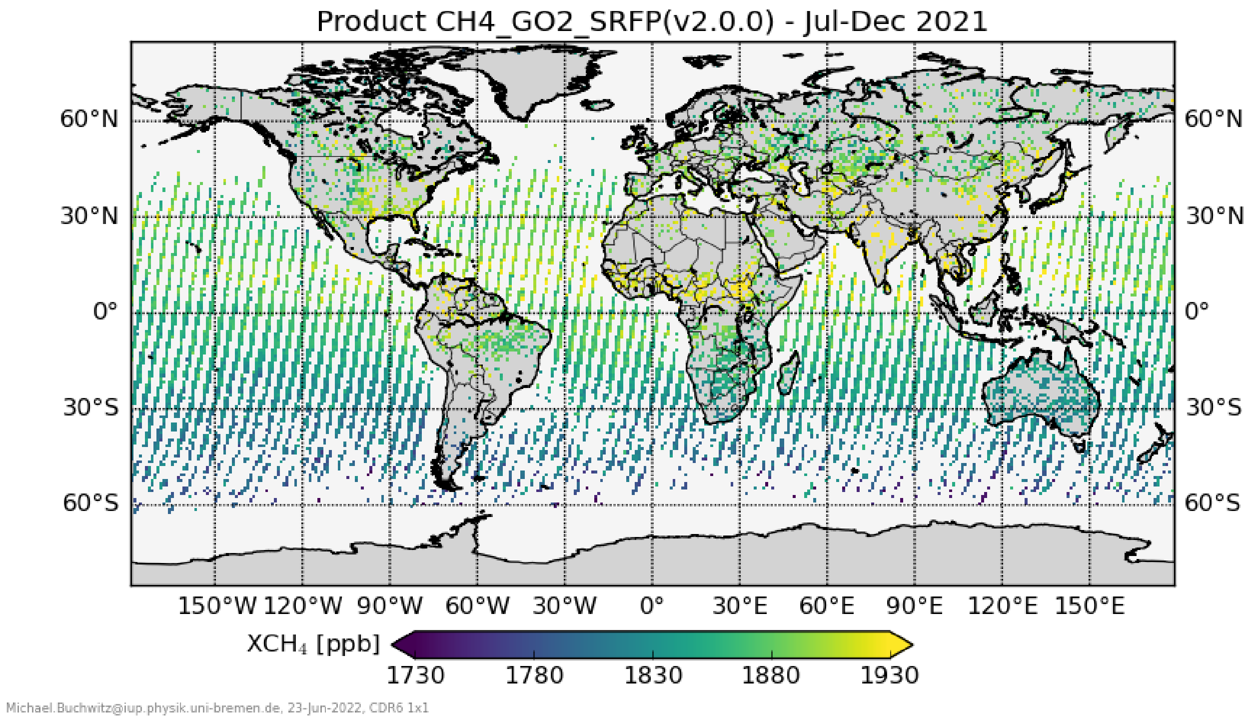
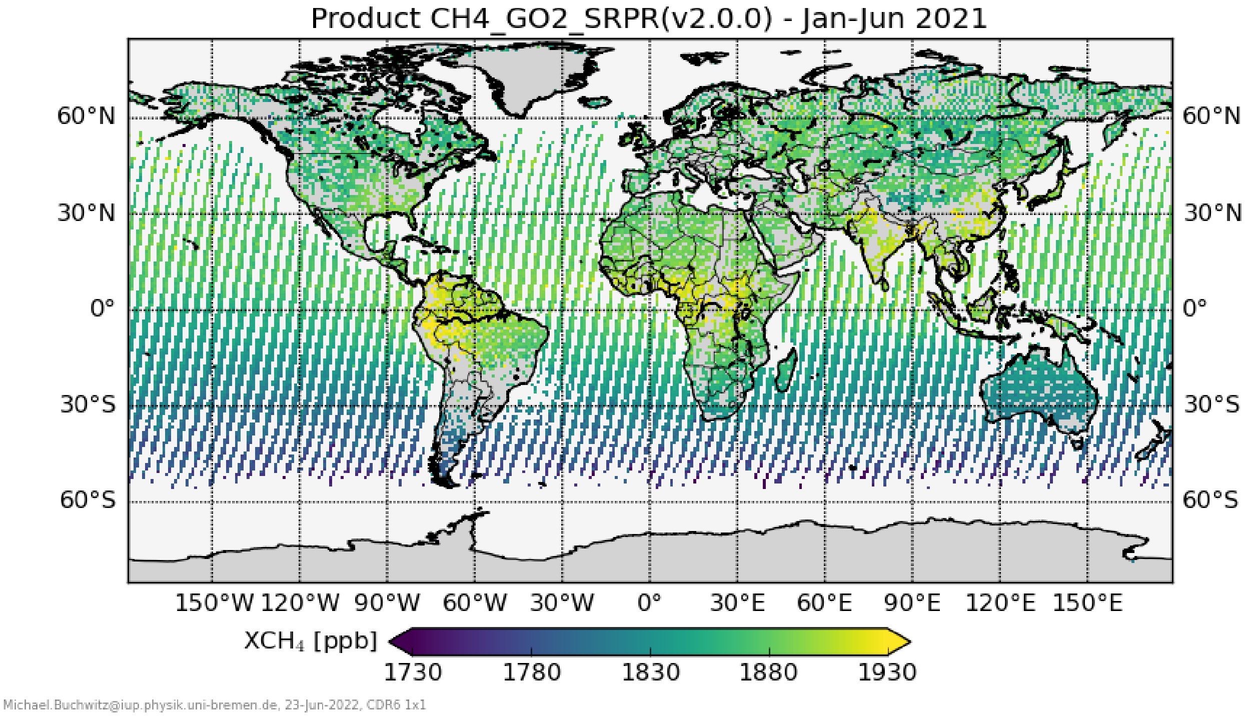
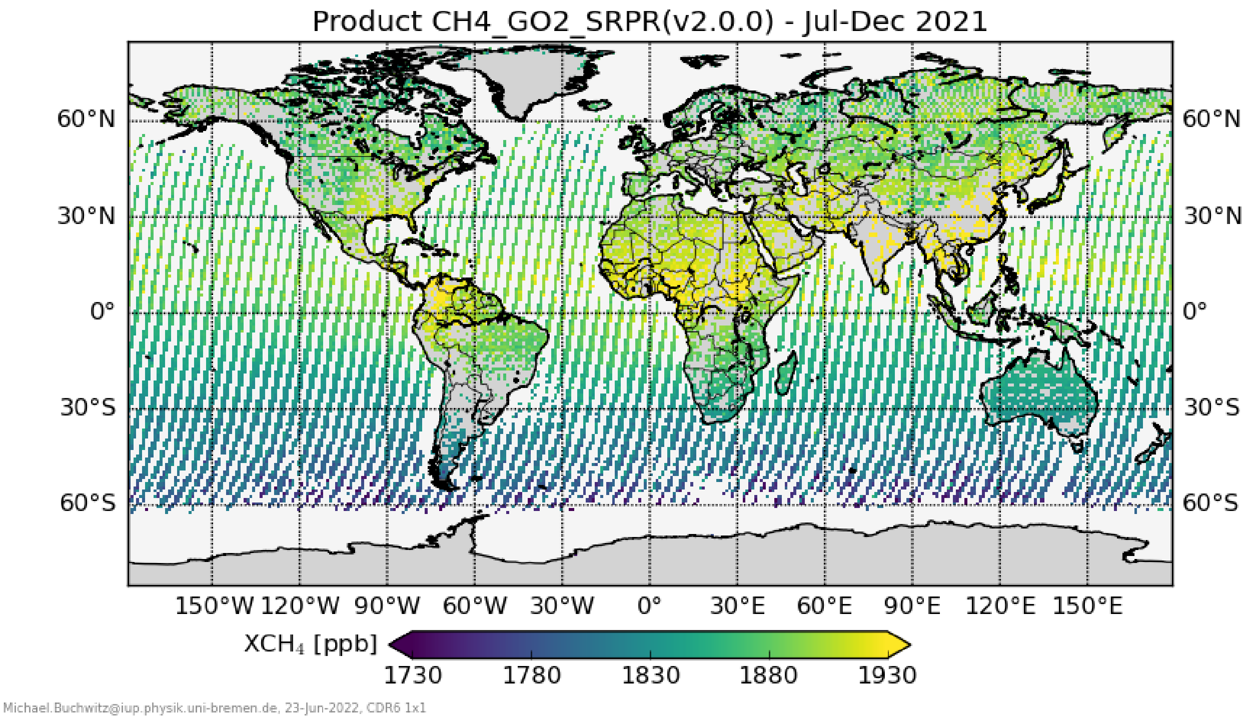


Figure 10 - XCH_4 product CH4_GO2_SRPR. Top: January to June 2021. Bottom: July – December 2021.





Latitude-time plots of products XCO2_EMMA and XCH4_EMMA are shown in Figure 11 and Figure 12, respectively. Discontinuities for «Uncertainty» and number of observations («Nobs») are due to the use of different satellites, which have - for example - different noise characteristics. Note that the product files contain all relevant information so that users can reproduce these figures.

Figure 11 – Latitude – time plot of XCO_2 product XCO2_EMMA.

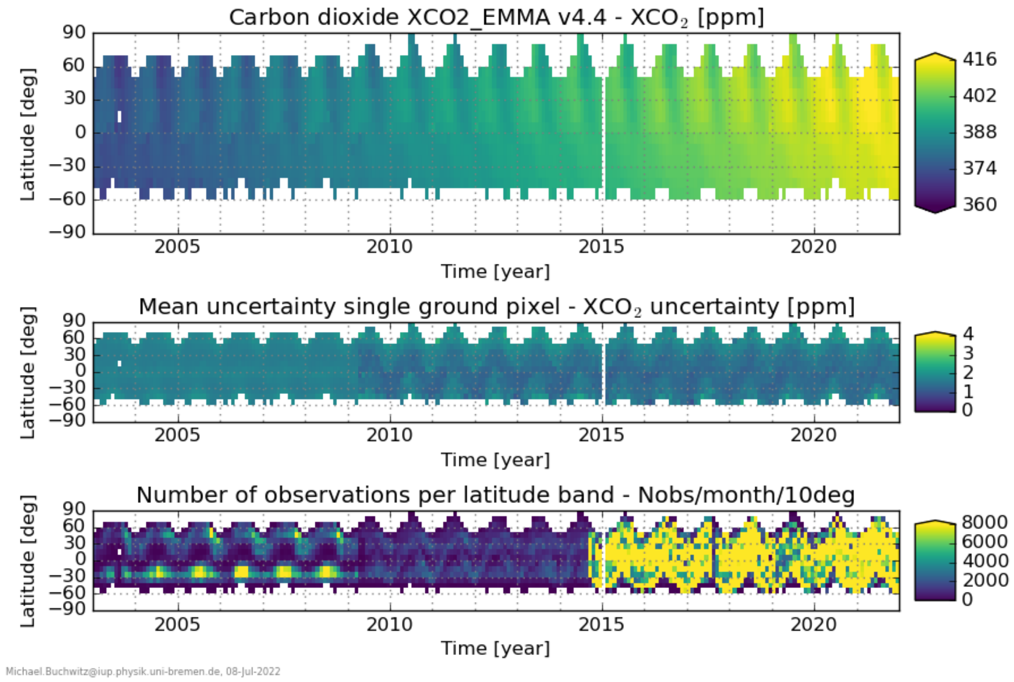
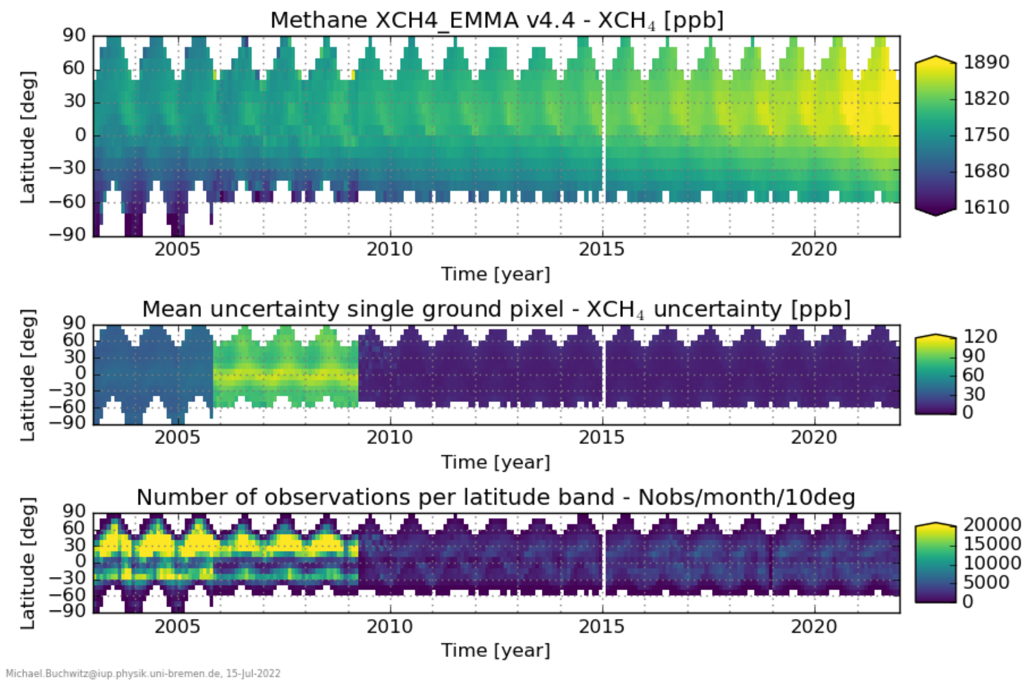


Figure 12 – Latitude – time plot of XCH_4 product XCH4_EMMA.



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 (down looking) observation viewing mode are sensitive to atmospheric CO_2 and CH_4 mixing ratio changes in the mid-tropospheric region. They can thus be interpreted in terms of integrated mid-tropospheric columns, with typical sensitivity between 5 and 12 km.

1.2.2 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 a 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).

As an example, Figure 13 shows time series of IASI/Metop-A derived mid-tropospheric CO_2 column as a function of time and latitude. The trend, seasonality and latitudinal gradient of CO_2 are clear in the figure. Figure 14 shows the same but for IASI/Metop-B.

Figure 15 and Figure 16 show spatial maps for the IASI/Metop-A and IASI/Metop-B products, respectively, to also illustrate the spatial coverage of the data for a typical month including number of observations and standard deviation.

Figure 13 – Monthly and latitudinal changes of mid-tropospheric CO_2 (top) as seen by IASI/Metop-A and number of observations per 10 deg latitude band (bottom).

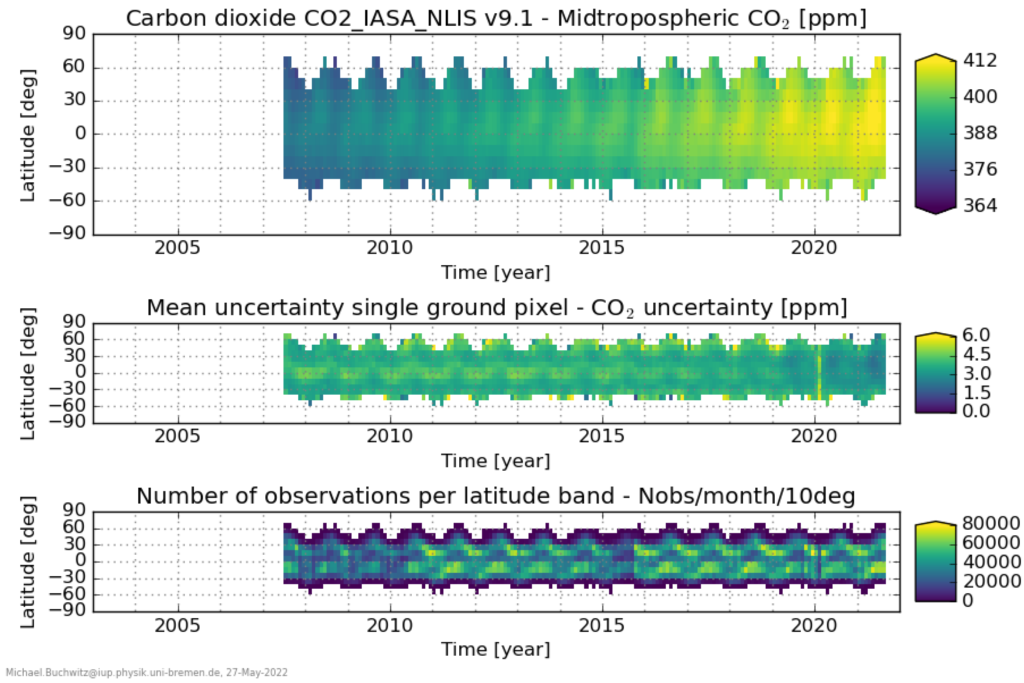


Figure 14 - Monthly and latitudinal changes of mid-tropospheric CO_2 (top) as seen by IASI/Metop-B and number of observations per 10 deg latitude band (bottom).

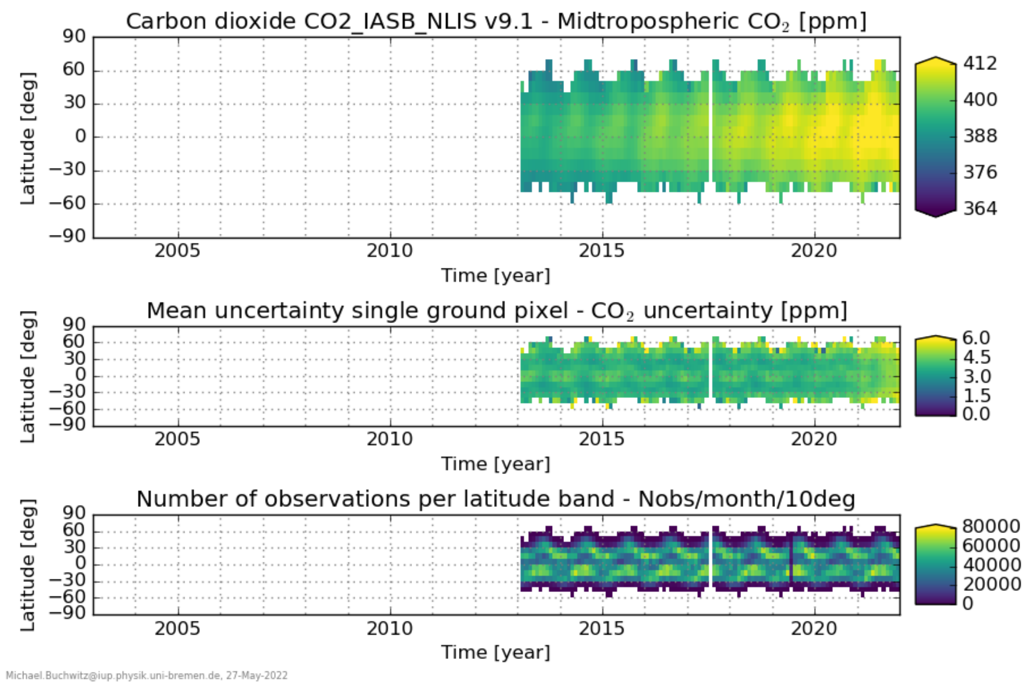


Figure 15 - Map of mid-tropospheric CO_2 from IASI/Metop-A for August 2021 (top left). Mean value of the reported uncertainty (top right), number of observations per 5°x5° grid size (bottom left) and standard deviation (bottom right).

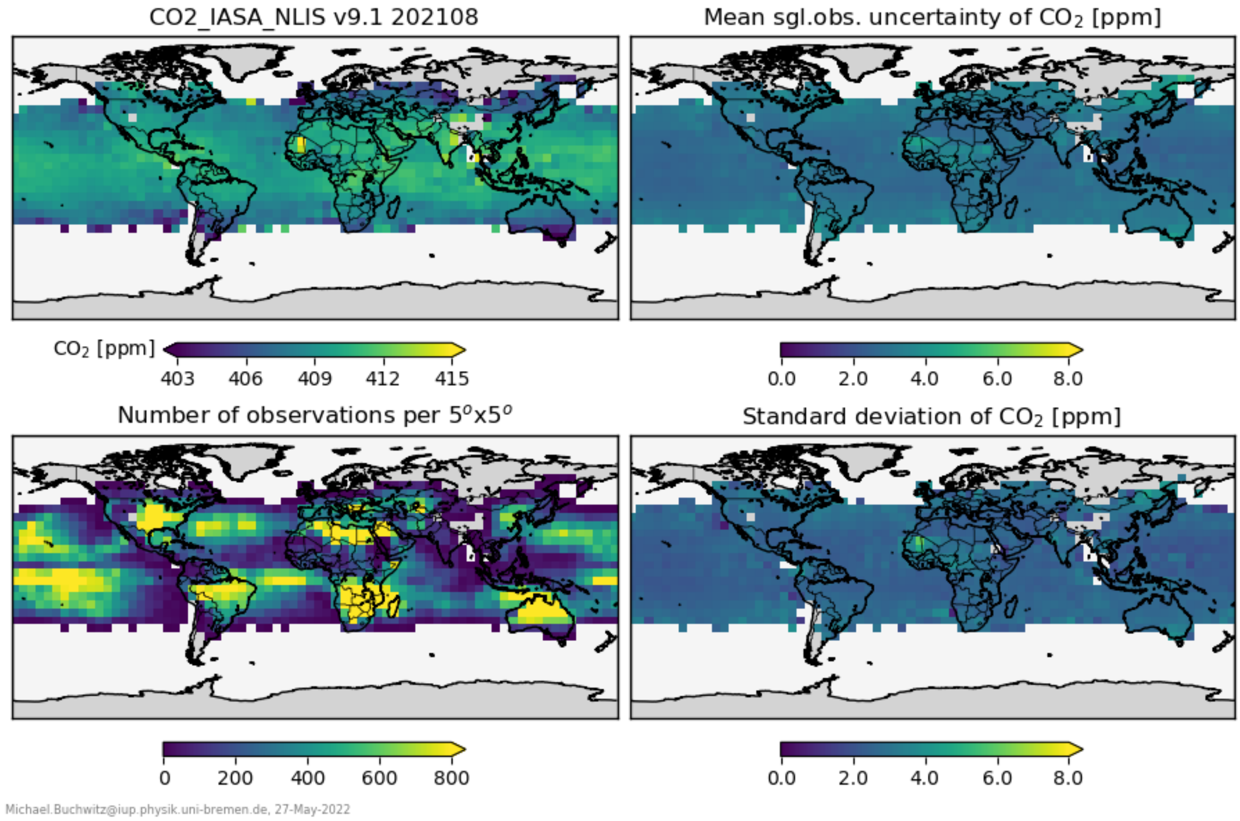
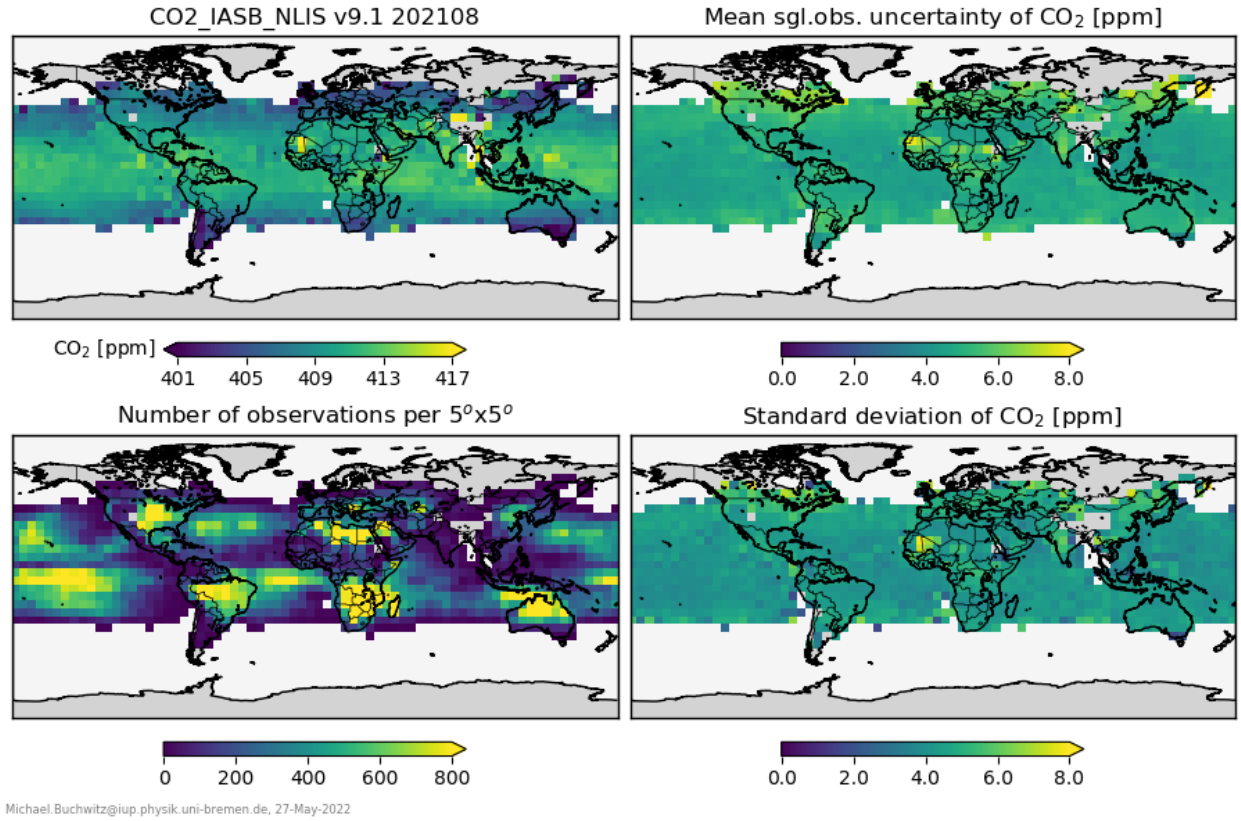


Figure 16 - Map of mid-tropospheric CO_2 from IASI/Metop-B for August 2021 (top left). Mean value of the reported uncertainty (top right), number of observations per 5°x5° grid size (bottom left) and standard deviation (bottom right).



1.2.3 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).

As an example, Figure 17 shows time series of IASI/Metop-A derived mid-tropospheric CO_2 column as a function of time and latitude. The trend, seasonality and latitudinal gradient of CO_2 are clear in the figure. Figure 18 shows the same but for IASI/Metop-B.

Figure 19 and Figure 20 show spatial maps for the IASI/Metop-A and IASI/Metop-B products, respectively, to also illustrate the spatial coverage of the data for a typical month including number of observations and standard deviation.

Figure 17 – Monthly and latitudinal evolution of mid-tropospheric CH_4 (top) as seen by IASI/Metop-A and number of observations per 10 deg latitude band (bottom).

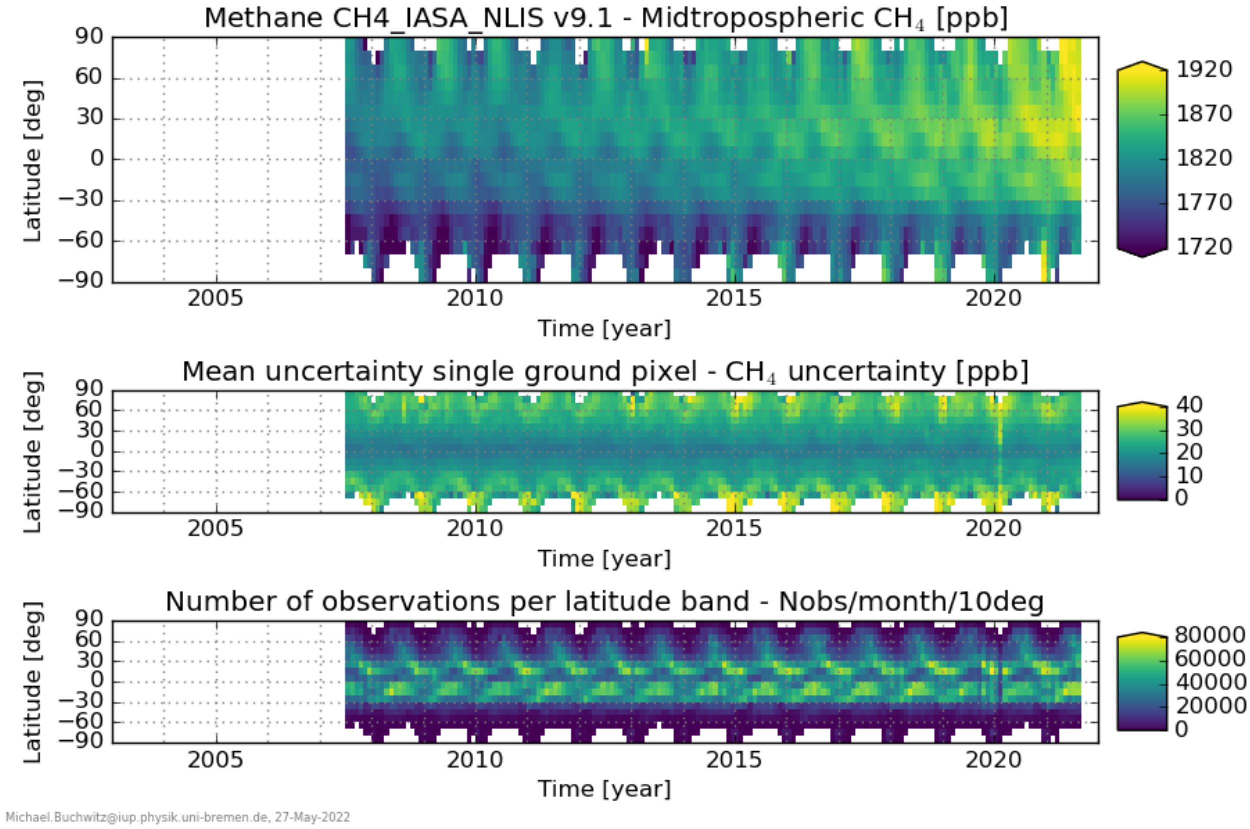


Figure 18 - Monthly and latitudinal evolution of mid-tropospheric CH_4 (top) as seen by IASI/Metop-B and number of observations per 10 deg latitude band (bottom).

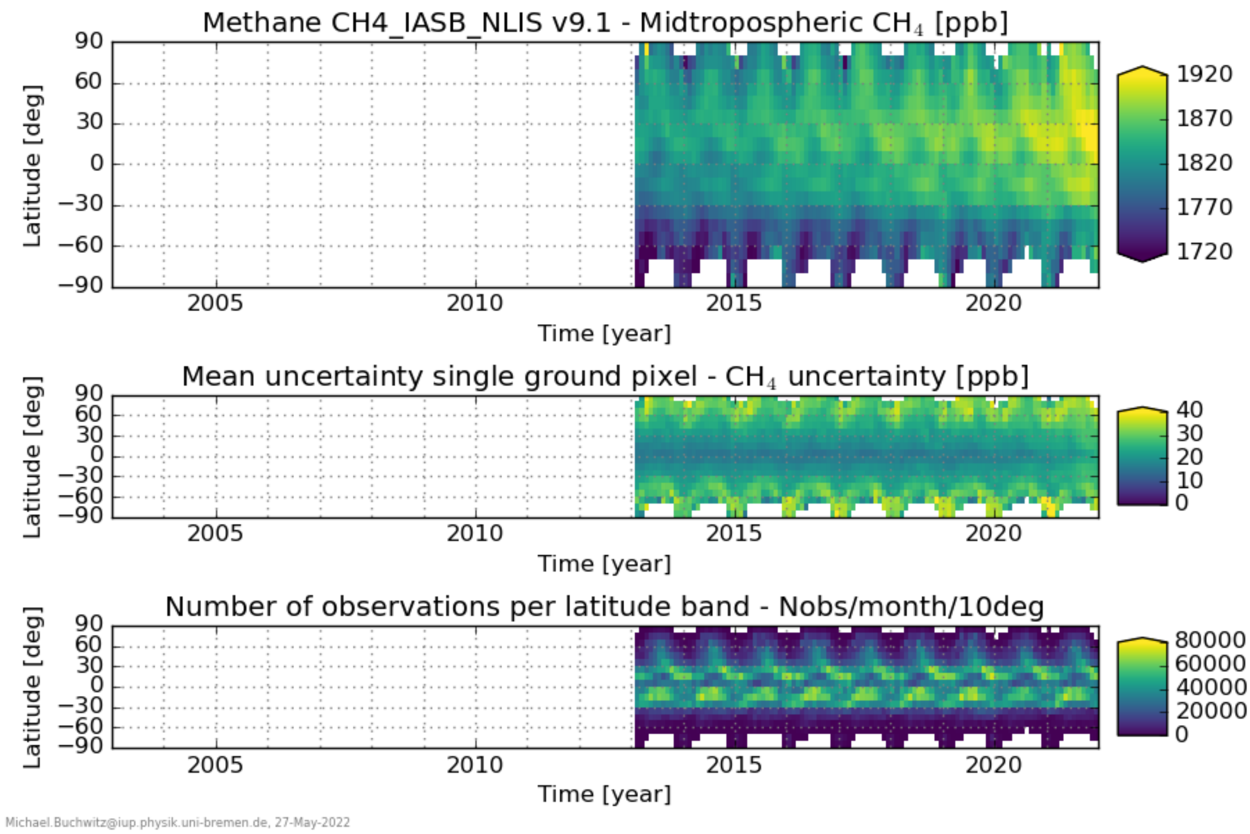


Figure 19 - Map of mid-tropospheric CH_4 from IASI/Metop-A for August 2021 (top left). Mean value of the reported uncertainty (top right), number of observations per 5°x5° grid size (bottom left) and standard deviation (bottom right).

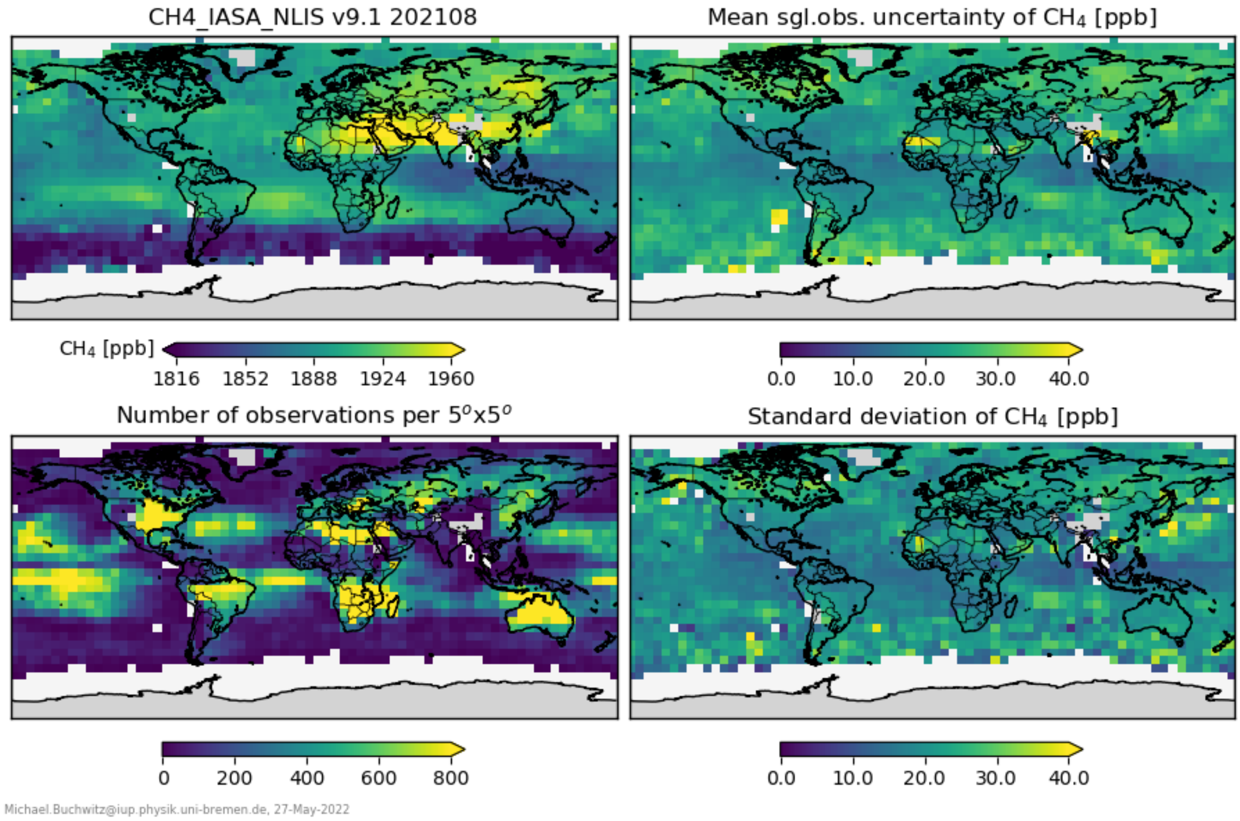
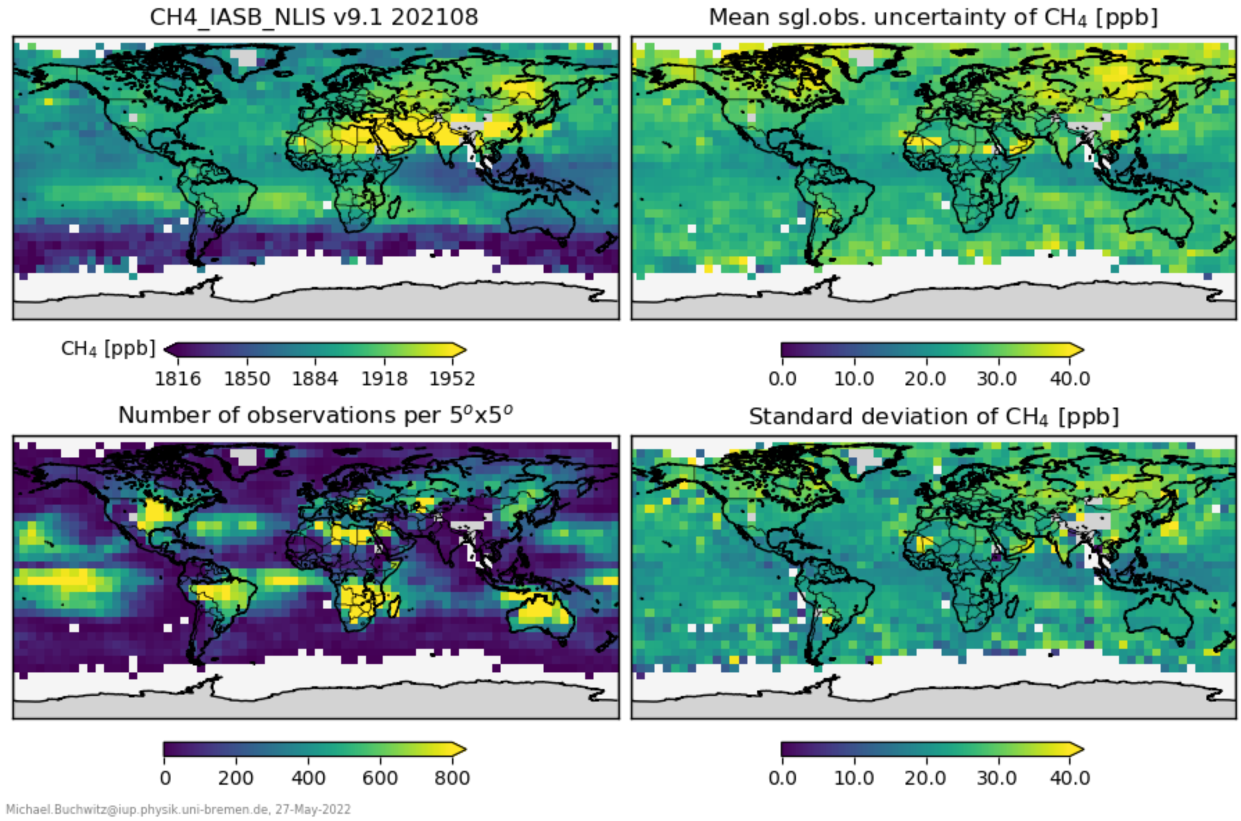


Figure 20 - Map of mid-tropospheric CH_4 from IASI/Metop-B for August 2021 (top left). Mean value of the reported uncertainty (top right), number of observations per 5°x5° grid size (bottom left) and standard deviation (bottom right).



1.2.4 List of mid-tropospheric CO_2 and CH_4 data products

Table 5 lists the CO_2 and CH_4 mid-tropospheric data products.

Table 5 - Overview mid-tropospheric CO_2 and CH_4 data products. CDR 5 refers to the previously generated "Climate Data Record" data set and CDR 6 refers to the new data set described in this document. Column "Availability" lists the (planned) date of availability of the data products in the Copernicus Climate Data Store[2] followed by the period covered by the corresponding product.

Product ID	Level	Sensor(s)	CDR: (Planned) Availability: Temporal coverage	Comments
CO2_IASA_NLIS	2	IASI / Metop-A	CDR 5: Jul. 2021: 2007 - 11.2020 CDR 6: Dec. 2022: 2007-07.2021	IASI-A: Nominal operation ended July 2021.
CH4_IASA_NLIS	2	IASI / Metop-A	CDR 5: Jul. 2021: 2007 – 11.2020 CDR 6: Dec. 2022: 2007-07.2021	IASI-A: Nominal operation ended July 2021.
CO2_IASB_NLIS	2	IASI / Metop-B	CDR 5: Jul. 2021: 2013 – 11.2020 CDR 6: Dec. 2022: 2013-2021	
CH4_IASB_NLIS	2	IASI / Metop-B	CDR 5: Jul. 2021: 2013 – 11.2020 CDR 6: Dec. 2022: 2013-2021	

[2] https://cds.climate.copernicus.eu (last access: 3-Apr-2023)

2. Level 2 XCO_2 and XCH_4 data products

2.1 Product description

The format of these data products is described in and compliant with the specification of the corresponding pre-cursor products as given in the GHG-CCI project Product Specification Document (PSD), version 3 (Buchwitz et al., 2014)[3]:

- Buchwitz, M., et al., ESA Climate Change Initiative (CCI) Product Specification Document (PSD) for the Essential Climate Variable (ECV) Greenhouse Gases (GHG), 6-June-2014, Version 3, 2014.

These products are in NetCDF-4 (classic) format and are in-line with CF (Climate and Forecasting) convention 3[4]. The products are essentially self-explaining in particular due to the metadata contained in each data product.

The file names start with the following string f ESACCI-GHG (to be consistent with the pre-cursor products), processing level (L2), product type (CO_2 or CH_4), sensor (e.g., SCIAMACHY, GOSAT), algorithm (e.g., BESD or SRFP), date (YYYYMMDD), file version (fv#) and file name extension (.nc), separated by hyphens ("-").
Examples:
ESACCI-GHG-L2-CO2-SCIAMACHY-BESD-20021216-fv1.nc
ESACCI-GHG-L2-CH4-GOSAT-SRFP-20120909-fv1.nc

Each *.nc product file corresponds to one day of satellite observations.

In *Buchwitz et al., 2014* the so-called Common Parameters of these products are described. These parameters are relevant for all users. In addition, each product may contain additional (algorithm specific) parameters, which are described in separate Product User Guides (PUGs).

For the C3S products a similar approach is used. In the following paragraphs the common parameters are described and the additional (algorithm specific) parameters are described in specific ANNEXes (see Sect. 7).

The description given in the following is applicable to the following C3S data products:

- CO2_GOS_OCFP
- CO2_GOS_SRFP
- CO2_GO2_SRFP
- CH4_GOS_OCFP
- CH4_GOS_SRFP

[3] https://www.iup.uni-bremen.de/carbon_ghg/docs/GHG-CCIplus/PSD/PSDv3_GHG-CCI_final.pdf (last access: 4-Apr-2023)

[4] https://cfconventions.org/cf-conventions/cf-conventions.html (last access: 3-Apr-2023)

- CH4_GOS_OCPR
- CH4_GOS_SRPR
- CH4_GO2_SRFP
- CH4_GO2_SRPR
- XCO2_EMMA
- XCH4_EMMA

2.1.1 Common parameters

In this section the common parameters of the XCO_2 and XCH_4 Level data products are described.

In order that these products can be used as easily as possible the aim has been to harmonize them. The goal was to make sure that users can easily switch from one product to another. This has been achieved for all products and parameters with the **exception** of the averaging kernels (describing the altitude sensitivity of the retrieved products) and related parameters. These parameters are closely related to retrieval algorithm specific characteristics and require special consideration by the users of these products as is explained in detail in Sect. 2.1.2.

Table 6 presents an overview of relevant XCO_2 and XCH_4 specific parameters (followed by a description of each) and their associated dimensions and details of shared parameters (i.e., parameters valid for both gases). The dimensions detailed in the table are defined as follows:

- ***n*****:** number of satellite observations (ground pixels) (per file, i.e., for the given day of observations)
- ***m*****:** number of atmospheric layers or levels
- ***k*****:** number of atmospheric levels

Dimensions ***m*** and ***k*** are used (only) for Averaging Kernels (AKs) and related parameters such as the CO_2 or CH_4 vertical profiles and corresponding profiles of “pressure weights” (see Sect. 2.1.2). As explained in Sect. 2.1.2, depending on product the provided AKs are either “layer-based AKs” or “level-based AKs”:

- For layer-based AKs, ***m*** is the number of layers, which are defined by ***k = m+1*** pressure levels (each layer is defined by an upper and lower pressure level).
- For level-based AK only levels are used, not layers. Here all vertical profiles have the same number of elements, namely ***m*** levels. Here the number of pressure levels is also ***m*** (i.e., ***k = m***).
- For more information on layer-based- and level-based AKs and their usage, please refer to Sect. 2.1.2 of this document.

Table 6: Description of Common Parameters of the XCO_2 and XCH_4 Level 2 data products.

Name	Type	Dimensions	Units	Short Description
Common parameters for XCO_2 products:				
xco2	Float	n	micromol per mol, abbreviated ppm, i.e., 10^{-6}	Retrieved column-averaged dry-air mole fraction of atmospheric carbon dioxide (XCO_2) in ppm.
xco2_uncertainty	Float	n	micromol per mol, abbreviated ppm, i.e., 10^{-6}	Statistical uncertainty of XCO_2 in ppm (1-sigma).
xco2_averaging_kernel	Float	n x m	[-]	XCO_2 averaging kernel (a profile = vector for each single observation). Quantifies the altitude sensitivity of the XCO_2 retrieval.
co2_profile_apriori	Float	n x m	micromol per mol, abbreviated ppm, i.e., 10^{-6}	A priori mole fraction profile of atmospheric CO_2 in ppm.
xco2_quality_flag	Byte	n	[-]	Quality flag for XCO_2 retrieval. 0=good.
Common parameters for XCH_4 products:				
xch4	Float	n	nanomol per mol, abbreviated ppb, i.e., 10^{-9}	Retrieved column-averaged dry-air mole fraction of atmospheric methane (XCH_4) in ppb.
xch4_uncertainty	Float	n	nanomol per mol, abbreviated ppb, i.e., 10^{-9}	Statistical uncertainty of XCH_4 in ppb (1-sigma)
xch4_averaging_kernel	Float	n x m	[-]	XCH_4 averaging kernel (a profile = vector for each single observation). Quantifies the altitude sensitivity of the XCH_4 retrieval.
ch4_profile_apriori	Float	n x m	nanomol per mol, abbreviated ppb, i.e., 10^{-9}	A priori mole fraction profile of atmospheric CH_4 in ppb.
xch4_quality_flag	Byte	n	[-]	Quality flag for XCH_4 retrieval, 0 = good.
Continued on next page …				

... continuation of table.

Name	Type	Dimensions	Units	Short Description
Common parameters for XCO_2 and XCH_4 products:				
solar_zenith_angle	Float	n	Degrees	Solar zenith angle
sensor_zenith_angle	Float	n	Degrees	Sensor zenith angle
time	Double	n	Seconds	Measurement time
longitude	Float	n	Degrees	Center longitude of the measurement
latitude	Float	n	Degrees	Center latitude of the measurement
pressure_levels	Float	n x k (note: k = m or k = m+1)	hPa	Vertical altitude coordinate in pressure units as used for averaging kernels
pressure_weight	Float	n x m	[-]	Pressure weights as used for averaging kernels

Description of each parameter:

xco2

Main XCO_2 parameter. Retrieved column-average dry-air mole fraction of atmospheric carbon dioxide (XCO_2) in ppm.

xco2_uncertainty

Statistical uncertainty of main XCO_2 parameter: 1-sigma uncertainty of the retrieved XCO_2 in ppm.

xco2_averaging_kernel

XCO_2 averaging kernel (for each observation: vertical profile = vector of dimension *m*).

Represents the sensitivity of the retrieved XCO_2 to atmospheric carbon dioxide mole fraction perturbations depending on pressure (height).

For details see Sect. 2.1.2.

co2_profile_apriori

A priori mole fraction profile of atmospheric carbon dioxide in ppm needed to apply the XCO_2 averaging kernels.

For details see Sect. 2.1.2.

xco2_quality_flag

Quality flag for XCO_2 retrieval. 0 = good. 1 = bad.

xch4

Main XCH_4 parameter. Retrieved column-average dry-air mole fraction of atmospheric methane (XCH_4) in ppb

xch4_uncertainty

Statistical uncertainty of main XCH_4 parameter: 1-sigma uncertainty of the retrieved XCH_4 in ppb.

xch4_averaging_kernel

XCH_4 averaging kernel (for each observation: vertical profile = vector of dimension *m*).

Represents the sensitivity of the retrieved XCH_4 to atmospheric methane mole fraction perturbations depending on pressure (height).

For details see Sect. 2.1.2.

ch4_profile_apriori

A priori mole fraction profile of atmospheric methane in ppb needed to apply the XCH_4 averaging kernels.

For details see Sect. 2.1.2.

xch4_quality_flag

Quality flag for XCH_4 retrieval. 0 = good. 1 = bad.

solar_zenith_angle

Solar zenith angle (SZA). Angle between the line of sight to the sun and the local vertical. SZA is a positive number (i.e., larger or equal to 0 deg).

sensor_zenith_angle

Sensor zenith angle is the angle between the line of sight from the observed ground pixel to the sensor and the local vertical. The sensor zenith angle is a positive number (i.e., larger or equal to 0 deg; 0 deg for exact nadir (downlooking) observation).

time

Measurement time in seconds since 01.01.1970 00:00:00.

longitude

Center longitude of the measurement. A number in the range -180 deg to +180 deg.
0 deg passes through Greenwich.

latitude

Center latitude of the measurement. A number in the range -90 deg (south pole) to +90 deg (north pole). 0 deg = equator.

pressure_levels

Pressure levels as used for the averaging kernels. Ordered from the bottom of the atmosphere to the top of the atmosphere (i.e., by decreasing pressure).

For details see Sect. 2.1.2.

pressure_weight

Layer / level dependent weights needed to apply the averaging kernels.

For details see Sect. 2.1.2.

Other parameters

Each product may contain additional parameters, see the product specific ANNEXes listed in Sect. 7.

2.1.2 How to use the averaging kernels (AK)?

2.1.2.1 Introduction

The averaging kernel describes the altitude sensitivity of the retrieval. It is defined as the ratio of the change of the retrieved quantity for a given change of the corresponding true quantity (note: averaging kernels are computed using a model atmosphere with known (=true) parameters).

For XCO_2 the averaging kernel is a vector (a one-dimensional array) which shows how the retrieved XCO_2 changes for a given change of the true XCO_2 due to a change of the true CO_2 profile at a given altitude (note: XCO_2 is computed from the CO_2 mixing ratio vertical profile taking into account the structure (e.g., finite number of layers / levels) of the underlying model atmosphere). In the ideal case the averaging kernel is 1.0 for all altitudes indicating perfect sensitivity for all altitudes. If the averaging kernel is 0.5 at a certain altitude, then this means that only 50% of a given enhancement at that altitude is retrieved (e.g., 0.5 ppm instead of 1 ppm). For XCH_4, the explanation is analogous.

In order to compare the satellite-retrieved XCO_2 and XCH_4 data products with model simulations and for inverse modelling of surface fluxes (see, e.g., *Bergamaschi el al., 2007*) the altitude sensitivity of the satellite retrievals has to be taken into account. Information on the altitude sensitivity is provided by the satellite XCO_2 and XCH_4 averaging kernels and corresponding CO_2 and CH_4 *a priori* vertical profiles.

For validation purposes the averaging kernels have to be considered in order to take the altitude sensitivity of the different instruments into account, see, e.g., *Wunch et al., 2010, 2011, Dils et al., 2013*.

All common variables described in Sect. 2.1.1 (e.g., xco2, xco2_uncertainty, time, longitude, etc.) can be used identically for all Level 2 products with the **exception** of the averaging kernels and related parameters, as these parameters are closely related to the underlying retrieval algorithm.

In this section how the averaging kernels and related parameters can be used is explained.

How these parameters have been defined depends on the retrieval algorithm used to generate a certain product and it was not possible to fully harmonize their use, i.e., their use depends on the product.

There are two different averaging kernel (AK) categories:
Depending on the product (and its underlying retrieval algorithm), the AKs are

- “layer-based” (IUP, Univ. Bremen, and SRON products) (see Sect. 2.1.2.3)

or

- “level-based” (Univ. Leicester products) (see Sect. 2.1.2.4).

In the following, more information on this is given including the information for which product which category is valid.

Note that the user can also determine "automatically" (or via inspection of the product files) which category a given product belongs to. For this purpose, the dimensions of the two variables pressure_levels and pressure_weight have to be compared:

- For "layer-based" products the vertical dimension of parameter **pressure_levels** is *m+1*, i.e., there is one entry more than for parameter **pressure_weight** (or any of the other parameters with a vertical dimension), which has *m* vertical entries, i.e., one entry less than parameter **pressure_levels**.
- For "level-based" products all parameters have *m* entries.

Important note:
The AK related parameters and how they can be used as described in this document is most interesting for users who want to use different products and prefer to easily switch from one product to another. The main purpose of the common parameters and methods described in this document is to provide the users with the parameters and formulas to do this. However, all products also contain additional parameters, not described in this document, but in the PUGS of the individual products (please see also the Algorithm Theoretical Basis Documents (ATBDs) of the individual algorithms used to generate the individual products). Using these additional parameters (and corresponding formulas) users may be able to obtain somewhat more accurate results (although the differences are expected to be very small).

2.1.2.2 Averaging kernel related parameters

For each single observation (ground pixel) six averaging kernel related parameters are contained in the satellite product files (see Table 7). How to use these parameters is described in the following two sub-sections Sect. 2.1.2.3 and Sect. 2.1.2.4.

Table 7: Overview of averaging kernel (AK) and related parameters. (*) The ground pixel dimension (*n*, see Table 6) is not listed here. Here each array is 1-dimensional (a vector of dimension *k* or *m*). Each element corresponds to one atmospheric level or layer as explained in Sect. 2.1.2.3 and Sect. 2.1.2.4.

Parameter Name	Mathematical symbol	Dimension (*)	Unit	Explanation
pressure_levels	*p*	*k*	[hPa]	Pressure levels; note: *k* = *m +1* (for layer-based approach) or *k* = *m* (for level-based approach)
pressure_weight	*pw*	*m*	[-]	Pressure weights for all layers / levels
xco2_averaging_kernel	*AK*	*m*	[-]	XCO_2 averaging kernel
co2_profile_apriori	*VMR*	*m*	µmol/mol, abbreviated ppm (10^{-6})	CO_2 *a priori* profile
xch4_averaging_kernel	*AK*	*m*	[-]	XCH_4 averaging kernel
ch4_profile_apriori	*VMR*	*m*	nanomol/mol, abbreviated ppb (10^{-9})	CH_4 *a priori* profile

2.1.2.3 How to use layer-based AKs?

This section describes how the common parameters related to averaging kernels (AKs) can be used to apply the satellite's AKs to model profiles in order to take the altitude sensitivity of the satellite's XCO_2 and XCH_4 retrievals into account.

Each product may (or may not) contain additional parameters and corresponding formulas, not described in this document (but in the corresponding PUG), which can be used to obtain somewhat more accurate results for a specific product (although the differences compared to the method described in this section are expected to be small).

For the layer-based approach the AKs and corresponding *a priori* CO_2 and CH_4 profiles are defined for layers and they correspond to layer averages. There are ***m*** layers, which are defined by ***k = m+1*** pressure levels.

The AK layer-based approach needs to be applied for the following products, i.e., to the University Bremen and SRON products):

- CO2_SCI_BESD
- CO2_GOS_SRFP
- CO2_GO2_SRFP
- XCO2_EMMA
- CH4_SCI_WFMD
- CH4_SCI_IMAP
- CH4_GOS_SRFP
- CH4_GOS_SRPR
- CH4_GO2_SRFP
- CH4_GO2_SRPR
- XCH4_EMMA

The layer-based approach is also described and used in *Bergamaschi et al., 2007*. Here a slightly modified version of their Eq. 2 is shown (here GHG = CO_2 or CH_4):

$$XGHG^{mod} = \sum_{i=1}^{m} \left[VMR_i^{apri} + AK_i (VMR_i^{mod} - VMR_i^{apri}) \right] pw_i \qquad \textbf{Eq. (1)}$$

- Here $XGHG^{mod}$ is the desired modelled XCO_2 or XCH_4 value, which corresponds to the satellite XCO_2 or XCH_4 retrievals.
- The sum is over the *m* atmospheric layers (located between pressure levels p_i and p_{i+1} with $i = 1...m$). Here pressure is the “normal” or “total” or “wet” pressure (not the “dry pressure”, see below). Here $i = 1$ corresponds to the bottom of the atmosphere and $i = k = m+1$ corresponds to the top of the atmosphere.
- pw_i is a layer-dependent weight (depending on algorithm/product, this corresponds to $\Delta p_i/p_{surf}$ of *Bergamaschi et al., 2007,* times a conversion factor for the conversion of wet to dry pressure).
- VMR_i^{apri} is the satellite *a priori* layer-averaged CO_2 or CH_4 volume mixing ratio (VMR) or, more precisely, Dry Mole Fraction (DMF), between pressure levels $p_i$and p_{i+1}(note: $p_i > p_{i+1}$).
- VMR_i^{mod} is the corresponding value of the model (CO_2 of CH_4) VMR (DMF) between pressure levels p_i and p_{i+1}.
- AK_i is the satellite XCO_2 or XCH_4 averaging kernel for layer *i*.

Note that in this equation all parameters are coming from the satellite product with the exception of VMR_i^{mod}.

Note that the described approach permits to use all satellite data as they are without the need to manipulate them, e.g., by interpolation. Only the model quantity VMR_i^{mod} needs to be computed.

Should a user wish to calculate $XGHG^{mod}$, the following procedure should be followed:

- For each satellite observation:
  - Interpolate the model profiles to the location and time of the satellite observation.
  - Compute for each satellite layer *i*, as defined by pressure levels p_i and p_{i+1}:
    - The layer-averaged model (CO_2 or CH_4) VMR (DMF), i.e., VMR_i^{mod}
  - Apply Eq. (1) to compute the desired quantity $XGHG^{mod}$.

Figure 21 and Figure 22 provide explanations how the parameters as provided via the satellite product files (Table 7) have to be used in order to apply Eq. (1).

Figure 21 - Overview of how to compute XCO_2 or XCH_4 (= XGHG) using the layer-based AK method. See also Figure 22.

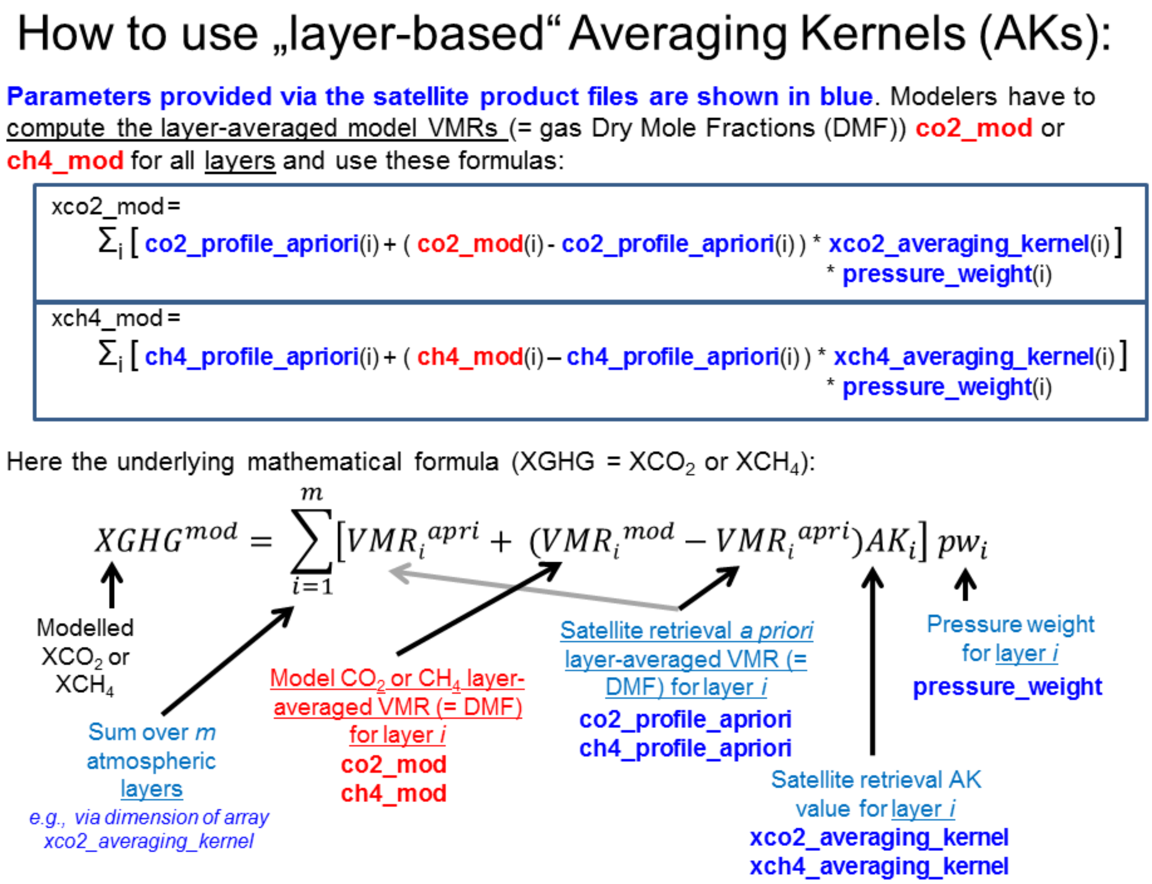
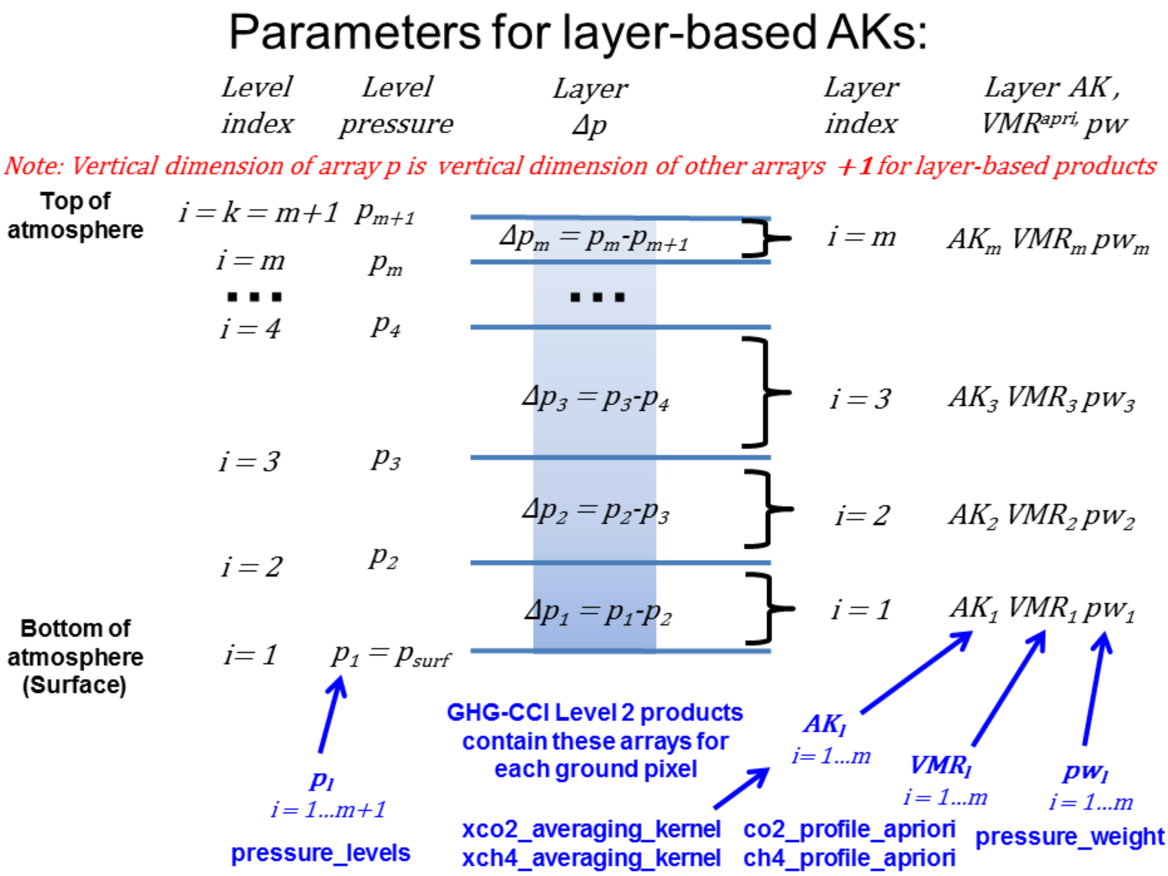


Figure 22 - Additional explanations related to the parameters needed to use the layer-based AK approach.



2.1.2.4 How to use level-based AKs?

For the level-based approach the AKs and corresponding a priori VMR (= DMF) profiles are defined on levels (not on layers).

The same parameters (variable names etc.) as provided via the satellite products files are used as for the layer-based approach described in the previous Sect. 2.1.2.3 but with a slightly different implementation to apply these parameters to compute the modelled XCO_2 or XCH_4.

For the level-based approach all AK related arrays are given for *m* levels.

The “AK level-based approach”, which is explained in this section, needs to be applied for the following GHG-CCI ECA products (all “OC” products):

- CO2_GOS_OCFP
- CH4_GOS_OCPR
- CH4_GOS_OCFP

For model comparisons and inverse modelling the following method is recommended in order to compute the modelled XCO_2 or XCH_4.

The equation to apply the level-based averaging kernels to the model data is the same as for the layer-based approach (Eq. 1) but with the variables now all on levels, rather than layers. The key point is that the model data (co2_mod or ch4_mod in Figure 23) must be interpolated onto the retrieval pressure levels (p_i). This interpolation should be done with care in order to conserve the total column amounts of *XGHG*.

Figure 23 and Figure 24 provide explanations how the parameters as provided via the satellite product files (Table 7) have to be used in order to apply Eq. (1).

Figure 23 - Overview how to compute XCO_2 or XCH_4 (= XGHG) using the level-based AK method. Additional explanations are given in Figure 24.

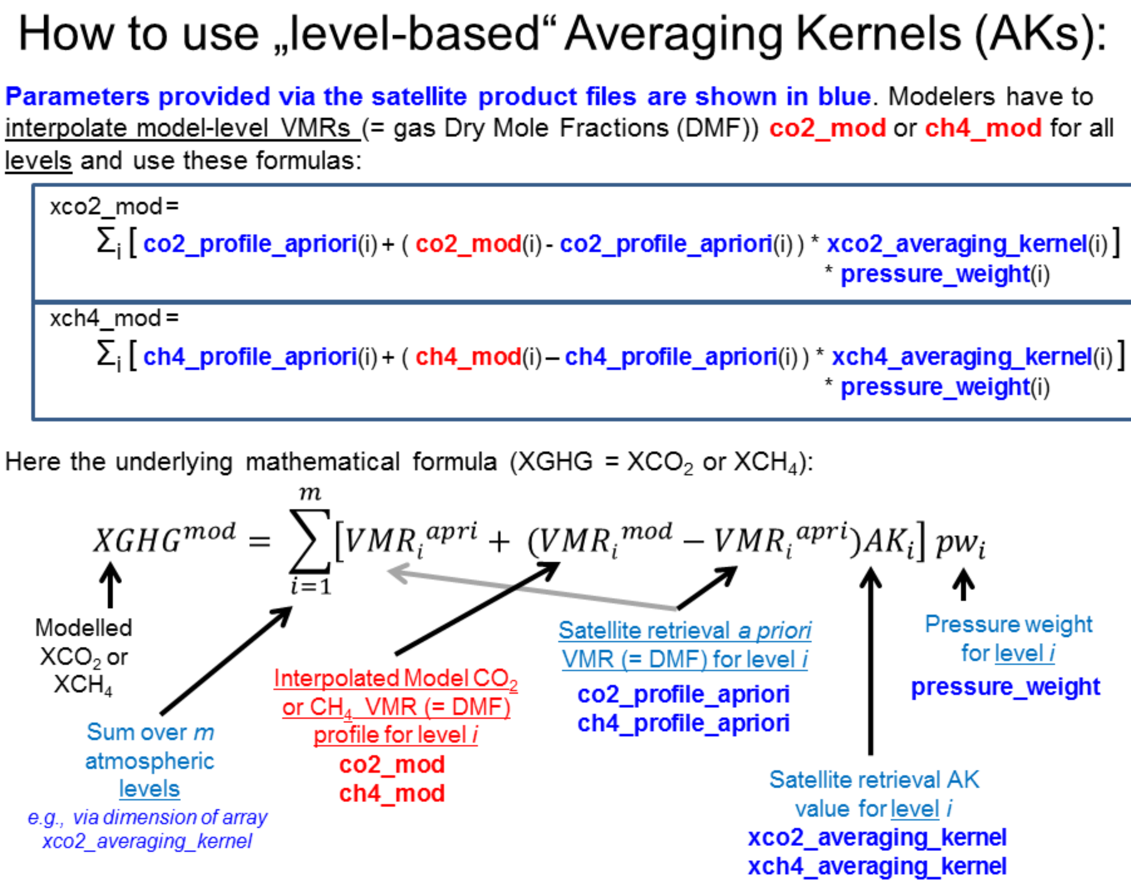
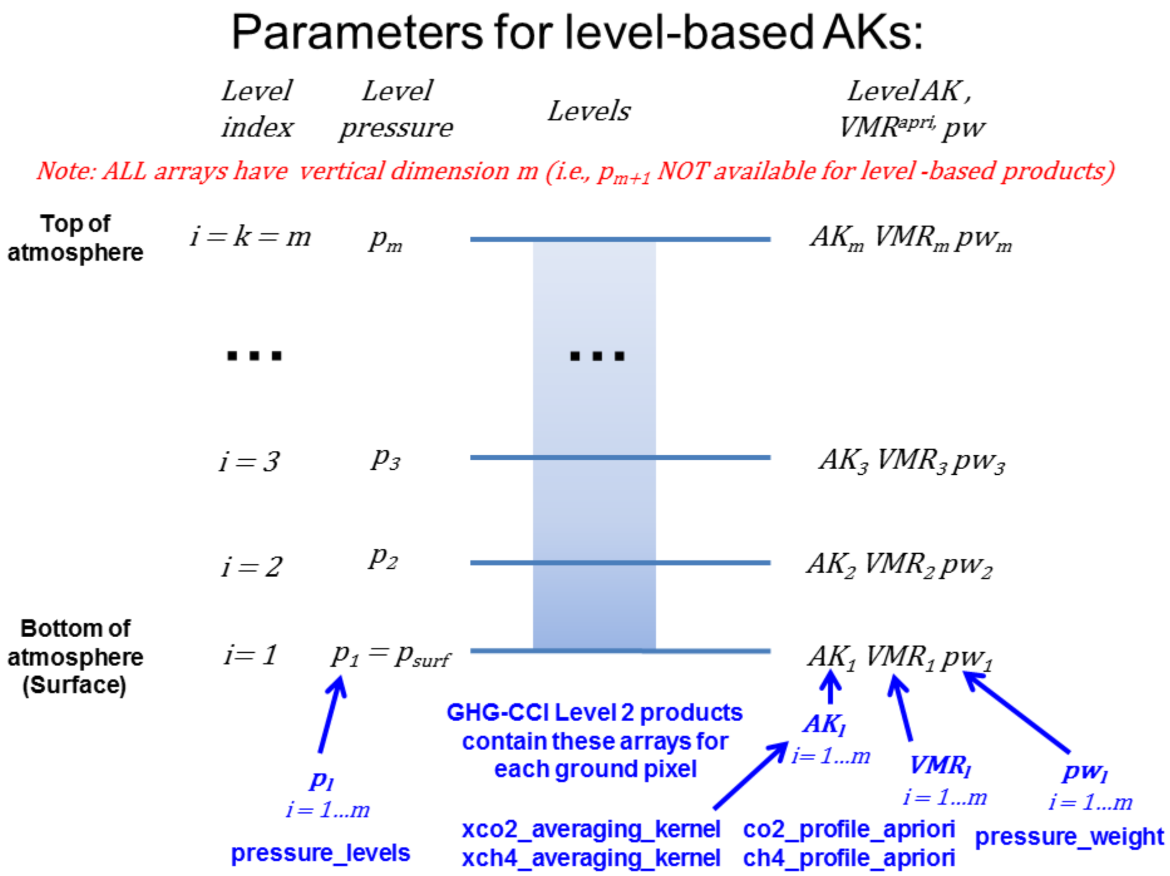


Figure 24 - Additional explanations related to the parameters needed to use the level-based AK approach.



2.2 Target requirements

2.2.1 Overview

Essential Climate Variables (ECVs) are defined by the Global Climate Observing System (GCOS) along with corresponding requirements (*D1, D2, D3, D6*). The ECV Greenhouse Gases (GHG) is defined by GCOS as follows: "Retrievals of greenhouse gases, such as CO_2 and CH_4, of sufficient quality to estimate regional sources and sinks" (*D1,* see their Table 2, product A.8.1).

Detailed Target Requirements (TR) for the ECV GHG products described in this document are provided in the Target Requirements and Gap Analysis Document (TRDGAD) (*D7*) and the corresponding quality assessment results are described in the corresponding Product Quality Assessment Report (PQAR) (*D9*). Here we provide a short summary referring for details to documents *D7* and *D9*.

The GCOS ECV GHG definition as given above essentially implies that the corresponding data products need to be useful for inverse modelling (or equivalent approaches) to derive information on regional scale sources and sinks, i.e., emissions and uptake or "surface fluxes" of CO_2 and CH_4. This implies that the satellite-derived CO_2 and CH_4 data products are sensitive to near-surface CO_2 and CH_4 concentration changes. This application implies high precision (low noise) and very good accuracy (low biases) of the satellite-derived data products as explained in *D7*. This application essentially also requires the generation of Level 2 products with latitude, longitude and time information for each single satellite retrieval (although some emission information can also be derived from averaged data (e.g., Buchwitz et al., 2017b)). These requirements therefore imply the generation of XCO_2 and XCH_4 Level 2 data products from satellite instruments with near-surface sensitivity such as SCIAMACHY/ENVISAT and TANSO-FTS/GOSAT as they measure reflected solar radiation in the near-infrared spectral region (permitting to extract appropriate XCO_2 and XCH_4 information). This is in contrast to instruments such as IASI measuring in the thermal infrared part of the electromagnetic spectrum with peak sensitivity in the middle or upper troposphere and typically only little near-surface sensitivity.

The focus of project C3S2_312a_Lot2 is therefore to generate Level 2 XCO_2 and XCH_4 products. However, in addition and as also described in this document, also other products are generated such as gridded (Level 3) XCO_2 and XCH_4 products and mid-tropospheric CO_2 and CH_4 products from IASI.

The focus of the following section is on the Level 2 XCO_2 and XCH_4 data products. Requirement related aspects for the Level 3 products are addressed in Sect. 3.2 and for the mid-tropospheric products in Sect. 4.2.

2.2.2 Required versus achieved performance of the Level 2 XCO_2 and XCH_4 products

The target requirements for the satellite-derived ECV XCO_2 and XCH_4 Level 2 products are provided in the Target Requirement and Gap Analysis Document (TRDGAD) (*D7*).

The TRDGAD (*D7*) requirements are based on GCOS requirements (*D1, D2, D3*), requirements as formulated by the Climate Modelling User Group (CMUG) of ESA's Climate Change Initiative (CCI) (*D5*) and requirements as formulated by the Climate Research Group (CRG) of the ESA GHG-CCI project (*D4*). The ESA GHG-CCI CRG requirements are highly relevant for the products as generated in this C3S2_312a_Lot2 project as these requirements consider the characteristics of existing satellite instruments, whereas the GCOS and CMUG requirements are less specific and often cannot be met by existing instruments. Examples are the 4 hour frequency requirement for tropospheric CO_2 or CH_4 columns as required by GCOS (see Table 23 from GCOS-200 (*D3*)). Neither can the frequency requirement be met with existing satellites nor has it been attempted to generate tropospheric column products (as none of the existing instruments has been designed for this). The latest GCOS requirements document GCOS-245 (*D6*) formulates requirements for XCO_2 and XCH_4 products (which is good) but for future satellite instruments and these requirements can also not be met using existing satellites. The TRDGAD (*D7*) requirements are therefore largely based on *D4*.

The spatial resolution of the generated Level 2 products is identical to the satellite footprint, i.e., depends only on the given satellite input data and is independent of the retrieval algorithm. A comparison of the achieved performance with the required performance is therefore not meaningful as spatial resolution is a given instrument characteristic. This is also true for temporal coverage and spatio-temporal sampling, which are also instrument characteristic. However, due to the demanding accuracy requirements (see below) the data need to be carefully filtered (flagged) to make sure that users get only data which are "good enough" or at least "as good as possible". Data filtering and quality flagging is part of the algorithms used to generate the data products. The challenge here is to achieve the highest possible yield meaning the largest amount of individual footprint data with as good as possible data quality. There is no explicit requirement on the fraction of footprints classified as "good". All retrieval teams aim at achieving a good compromise between amount of data and accuracy.

Spatio-temporal characteristics of the satellites instruments we are using are as follows:

- SCIAMACHY/ENVISAT: 60 km cross-track and 30 km along-track in nadir mode; swath width 960 km; but nadir mode only about 50% of the time due to other observations modes (especially limb observations)
- GOSAT and GOSAT-2 products: 10 km (diameter); the single observations are typically on the order of 100 km apart
- OCO-2: 1.29 km cross-track and 2.25 km along-track; swath width 10 km

The most important requirements (which are related to retrieval algorithms and not to given instrument characteristics) for the envisaged applications are the random and systematic error requirements and the stability requirements.

The TRDGAD (*D7*) document contains explicit requirements for random errors, systematic errors and stability of the XCO_2 and XCH_4 data products in terms of goal (G), breakthrough (B) and threshold (T) requirements. The relevant table from *D7* is shown here as Table 8.

In the following, a short overview of the achieved data quality is given. For details users should consult document PQAR (*D9*). That document also contains a detailed description of the methods used to obtain the quality assessment results summarized here.

The achieved performance for the Level 2 XCO_2 and XCH_4 products is shown in Figure 25 and Figure 26, respectively. Assessment results are presented for (i) "Single measurement random error" (often also referred to as "Retrieval precision"), (ii) accuracy and (iii) stability.

As can also be seen from these two figures, more than one comparison method has been used to obtain the assessment results for a given product. This has been done to enhance the robustness of the conclusions. Therefore, more than one vertical bar is shown for the different products in these two figures (for details please see *D9*).

Level 2 products are single observation products and results are reported per ground-pixel (per footprint). The relevant requirements for "Random error" are therefore those listed in column "Single obs." in Table 8. The achieved performance is shown in the top panel of Figure 25 for XCO_2 and in the top panel of Figure 26 for XCH_4.

The following can be concluded by comparing the requirements listed in Table 8, with the achieved performance for XCO_2 shown in Figure 25 and the achieved performance for XCH_4 shown in Figure 26:

The achieved performance in terms of random errors is typically better than the B requirement (< 3 ppm) for XCO_2 and close to the B requirement (< 17 ppb) for XCH_4, except for the SCIAMACHY XCH_4 products, where random errors are even exceeding the T requirement (34 ppb) (due to detector related issues resulting in quite noisy retrievals especially after 2005).

The most demanding requirement is the systematic error requirement, which is "better than 0.5 ppm" (threshold (T) requirement) for XCO_2 and "better than 10 ppb" (T requirement) for XCH_4 (see Table 8). Especially for XCO_2 this requirement is hardly achievable with current satellite sensors and one has to note that also ground-based reference data as used for validation are not much better than 0.5 ppm (see *D9* for details).

For accuracy and stability, the achieved performance is shown in Figure 25 and Figure 26 but also in addition the probability that the corresponding threshold requirement is met. The probabilities have been computed taking into account the uncertainty of the reference data and the uncertainty of the comparison method (see document *D9* for details).

The results for the achieved accuracy are shown in the second and third panels of the two figures. The absolute values of the achieved accuracy are shown in the 2nd panel of each figure. The achieved accuracy (or bias) has been estimated by comparisons with ground-based reference data (see *D9*). The lowest value of a vertical bar corresponds to the spatial bias and the upper value corresponds to the spatio-temporal bias (obtained by quadratically adding the temporal bias to the spatial bias). The dotted horizontal line shows the threshold (T) requirement (for XCH_4 in Figure 26 also a second line is shown indicating the breakthrough (B) requirements). The 3rd panel shows the corresponding probabilities.

From the 2nd panel of Figure 25 it can be seen that the spatio-temporal XCO_2 bias nearly always (i.e., for nearly all products and all assessment methods) exceeds the accuracy requirement of 0.5 ppm. As can be seen from the 3rd panel, the probability that this 0.5 ppm requirement is met is at best 77% (for the XCO2_EMMA product) but worse for the other products (the probability can be as low as 21% for the new GOSAT-2 product CO2_GO2_SRFP).

From the 2nd panel of Figure 26 it can be seen that the spatio-temporal biases of the various XCH_4 products are (depending on assessment method) typically better than the threshold requirement of 10 ppb except for the SCIAMACHY products. The probability that the threshold requirement is met is in the range 74% - 90% except for the SCIAMACHY products (55%-62%).

The two panels at the bottom of the two figures show the corresponding results for stability. As can be seen, the stability of nearly all products is good (often larger than 90%).

Finally, here a summary of the quality assessment results:

XCO_2 Level 2 products (see D9):

Figure 25 shows a summary of the achieved performance in terms of single measurement random error (precision), relative accuracy or systematic error in terms of spatial (lower value) and spatio-temporal (higher value) biases (i.e., neglecting a possible constant bias or global offset) and stability in terms of linear bias drift/trend as obtained from comparison with TCCON XCO_2. Note that this figure contains for completeness results from previous assessments for CDR5 for products not updated for CDR6. These products are: SCIAMACHY products and SRON GOSAT products. See corresponding CDR5 documents (ATBD GHG, 2021; PQAR GHG, 2021; PUGS GHG, 2021).

XCH_4 Level 2 products (see D9):

Figure 26 shows a summary of the achieved performance in terms of single measurement random error (precision), relative accuracy or systematic error in terms of spatial (lower value) and spatio-temporal (higher value) biases (i.e., neglecting a possible constant bias or global offset) and stability in terms of linear bias drift/trend as obtained from comparison with TCCON XCH_4. Note that this figure contains for completeness results from previous assessments for CDR5 for products not updated for CDR6. These products are: SCIAMACHY products and SRON GOSAT products. See corresponding CDR5 documents (ATBD GHG, 2021; PQAR GHG, 2021; PUGS GHG, 2021).

Comparison of required performance with achieved performance:

As an overall summary, Table 9 presents and overview of the required performance for random and systematic error and stability with the achieved performance for the Level 2 XCO_2 and XCH_4 data products as generated in this project.

Table 8: XCO_2 and XCH_4 random ("precision"), systematic error and stability requirements (from *D7*). Abbreviations: G=Goal, B=Breakthrough, T=Threshold requirement. §) Required systematic error after an empirical bias correction, that does not use the verification data. #) Required systematic error and stability after bias correction, where bias correction is not limited to the application of a constant offset / scaling factor.

Random and systematic error requirements for XCO_2 and XCH_4					
Parameter	**Req. type**	**Random error** ("Precision")		**Systematic error**	**Stability**
		Single obs.	1000^2 km^2 monthly		
XCO_2	G	< 1 ppm	< 0.3 ppm	< 0.2 ppm (absolute)	As systematic error but per year
	B	< 3 ppm	< 1.0 ppm	< 0.3 ppm (relative §))	-"-
	T	< 8 ppm	< 1.3 ppm	< 0.5 ppm (relative #))	-"-
XCH_4	G	< 9 ppb	< 3 ppb	< 1 ppb (absolute)	< 1 ppb/year (absolute)
	B	< 17 ppb	< 5 ppb	< 5 ppb (relative §))	< 2 ppb/year (relative §))
	T	< 34 ppb	< 11 ppb	< 10 ppb (relative #))	< 3 ppb/year (relative #))

Figure 25 - Overview data quality assessment results for Level 2 XCO_2 data products (from D9). The green bars refer to the "Quality Assessment / Quality control" (QA/QC) results as described in detail in document D9. The red bars refer to results obtained by the data providers (DPs) (see D9). 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 Requirement (TR) assessments. The listed values for products generated in previous C3S projects (products CO2_SCI_BESD, CO2_SCI_WFMD and CO2_GOS_SFFP) are listed here for completeness but have not been updated (for details see D9).

Figure 26 - Overview data quality assessment results for Level 2 XCH_4 data products (from *D9*). The green bars refer to the "Quality Assessment / Quality control" (QA/QC) results as described in detail in document *D9*. The red bars refer to results obtained by the data providers (DPs) (see *D9*). 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 Requirement (TR) assessments. The listed values for products generated in previous C3S projects (products CH4_SCI_WFMD, CH4_SCI_IMAP, CH4_GOS_SRFP and CH4_GOS_SFPR) are listed here for completeness but have not been updated (for details see *D9*).

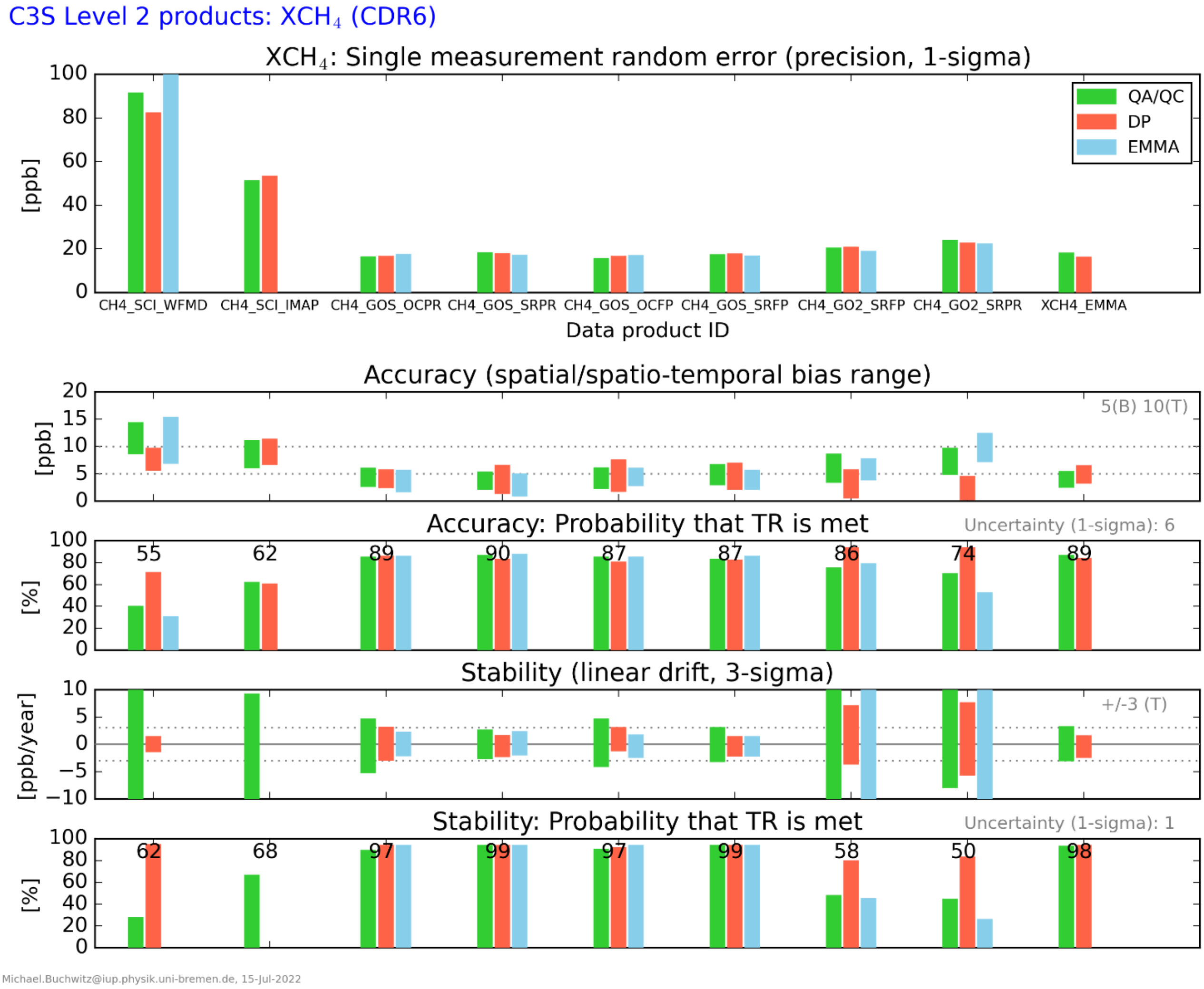


Table 9: Comparison of required performance (see *D7*) with achieved performance in terms of probability that the corresponding requirement is met (see *D9*). Listed are only products as generated in this project. (#) Achieved performance in mixing ratio units in brackets.

	Random error single observation	Systematic error (spatio-temporal bias)	Stability (linear bias drift)	Comment
	Level 2 XCO_2 products:			
Required (T)	**< 8 ppm (#)**	**< 0.5 ppm**	**< 0.5 ppm/year**	
Achieved:	Probability that threshold requirement is met:			
CO2_GOS_OCFP	100% (2.0 ppm)	44%	96%	
CO2_GOS_SRFP	100% (2.2 ppm)	44%	97%	
CO2_GO2_SRFP	100% (2.6 ppm)	21%	61%	
XCO2_EMMA	100% (1.8 ppm)	77%	96%	
	Level 2 XCH_4 products:			
Required (T)	**< 34 ppb (#)**	**< 10 ppb**	**< 3 ppb/year**	
Achieved:	Probability that threshold requirement is met:			
CH4_GOS_OCPR	100% (18 ppb)	89%	97%	
CH4_GOS_OCFP	100% (18 ppb)	87%	97%	
CH4_GO2_SRPR	100% (20 ppb)	86%	58%	
CH4_GO2_SRFP	100% (20 ppb)	74%	50%	
XCH4_EMMA	100% (16 ppb)	89%	98%	

2.3 Data usage information

The data format is described in detail in Sect. 2.1.

As explained in that section, the main variables are xco2 (in ppm) and xch4 (in ppb). Also reported are the corresponding (1-sigma) uncertainties (variables xco2_uncertainty (in ppm) and xch4_uncertainty (in ppb)). Important is also the quality flag (variables xco2_quality_flag and xch4_quality_flag). For “good” data the numerical value of the quality flag is 0 (zero). All results shown in this document (and in other documents such as *D9* presenting the validation and comparison results) are for “good” data with quality flag = 0. All Level 2 product contain this variable but some only contain “good” data. It is strongly recommended to use this variable and to use only data with quality flag = 0.

These variables are reported per satellite footprint along with spatial (variables latitude and longitude) and temporal information (variable time). The latitudes and longitudes are the footprint centre coordinates. This information is provided for all Level 2 data products (see common variables in Sect. 2.1.1). The individual satellite data products may contain additional information such as footprint corner coordinates (see the product specific Annexes to this main PUGS document as listed in Sect. 7). Furthermore, for each footprint additional information is provided such as averaging kernels and *a priori* profiles (see Sect. 2.1).

Note that use of the atmospheric CO_2 and CH_4 data products is not trivial and typically the interpretation of these products requires appropriate modelling. The main reason for this is the long lifetime of CO_2 and CH_4 in the atmosphere combined with atmospheric transport (and for CH_4 also atmospheric chemistry needs to be considered). As a consequence, atmospheric concentrations may be locally or regionally higher (or lower) compared to background concentration far away from the source (or sink) region. A further complication arises due to the sparseness of the data due to the spatial coverage of the satellite data, because measurements can only be made on parts of the dayside (the solar zenith angle must be smaller than about 75^o) but also because of cloud contamination and other reasons (e.g., contamination due to desert dust).

The data products described can be used in combination with appropriate modelling to obtain information on the various natural and anthropogenic surface sources and sinks of CO2 and CH4 as shown in a number of scientific publications such as Alexe et al., 2015; Bergamaschi et al., 2009, 2013; Detmers et al., 2015; Guerlet et al., 2013; Houweling et al., 2004, 2015; Pandey et al., 2016; Reuter et al., 2014a, 2014b, 2017; Ross et al., 2013; Schneising et al., 2014a, 2014b; Turner et al., 2015, 2016. They can also be used for comparisons with models (e.g., carbon models or global chemistry-climate models) as also shown in a number of publications such as Buchwitz et al., 2005, 2013; Cogan et al., 2011; Hayman et al., 2014; Parker et al., 2011; Shindell et al., 2013. The products can also be used to study atmospheric trends and variability as shown in Buchwitz et al., 2007; Frankenberg et al., 2011; Schneising et al., 2011. For a comprehensive list of relevant publications including links to these publications please see the publication list on the ESA GHG-CCI project website. Note that all satellite-derived CO_2 and CH_4 products generated now operationally via C3S (as described in this document) have initially been (further) developed as part of the ESA GHG-CCI project, which focussed on the needed research and development activities to make algorithms fit for operational purposes.

The products do not have any known issues.

3. Level 3 XCO_2 and XCH_4 data products

3.1 Product description

The Level 3 data products are in Obs3MIPs format and described in Sect. 3.1.1 for XCO_2 and in Sect. 3.1.2 for XCH_4. Obs4MIPs (Observations for Model Intercomparisons Project)[5]) is an activity to make observational products more accessible especially for climate model intercomparisons.

The XCO_2 and XCH_4 Obs4MIPs products are gridded data products with a spatial resolution of 5°x5° (i.e., using an equirectangular (Cartesian) latitude/longitude grid) and monthly time resolution. These products have been generated using as input the Level 2 EMMA products described in Sect. 2 and in more detail in ANNEX D (see Sect. 7.4).

We also recommend that users of these Level 3 products should read the relevant peer-reviewed publication, i.e., Reuter et al., 2020, describing how (a previous version of) this data product has been generated and how it can be used to address scientific applications.

Figure 27 to Figure 30 show examples of these products in terms of XCO_2 and its uncertainty and XCH_4 and its uncertainty for selected months as directly contained in the product files.

[5] https://www.earthsystemcog.org/projects/obs4mips/ (last access: 3-Apr-2023)

Figure 27 –OBS4MIPS XCO_2 (left) and corresponding uncertainty (right) for August 2003.

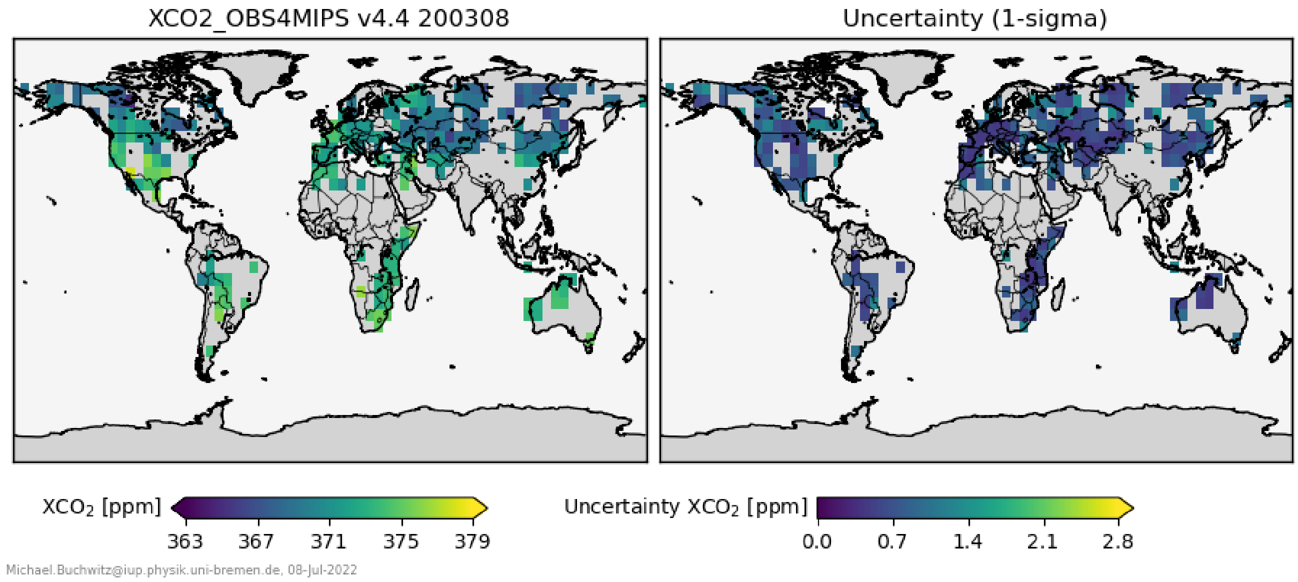


Figure 28 – OBS4MIPS XCO_2 (left) and corresponding uncertainty (right) for August 2021.

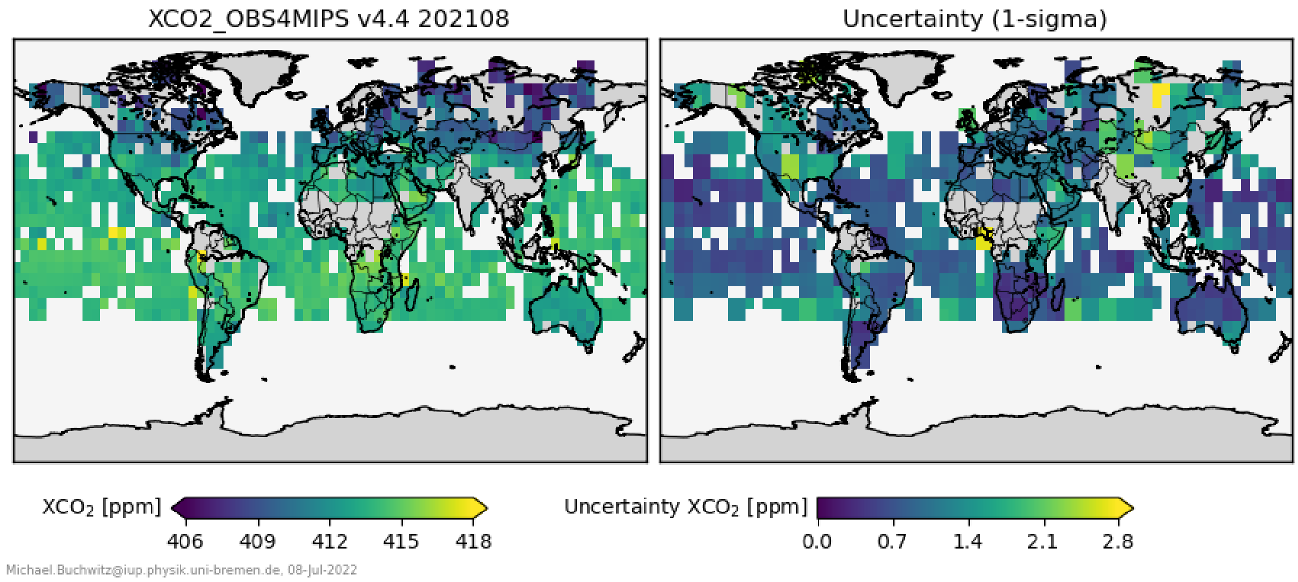


Figure 29 –OBS4MIPS XCH_4 (left) and corresponding uncertainty (right) for August 2003.

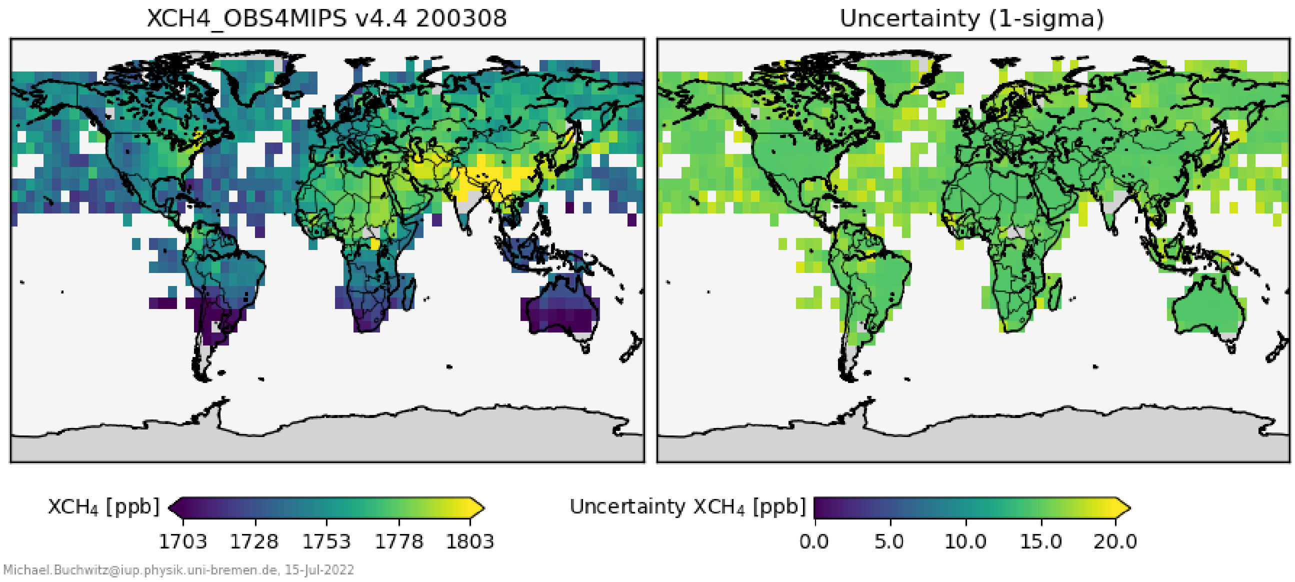
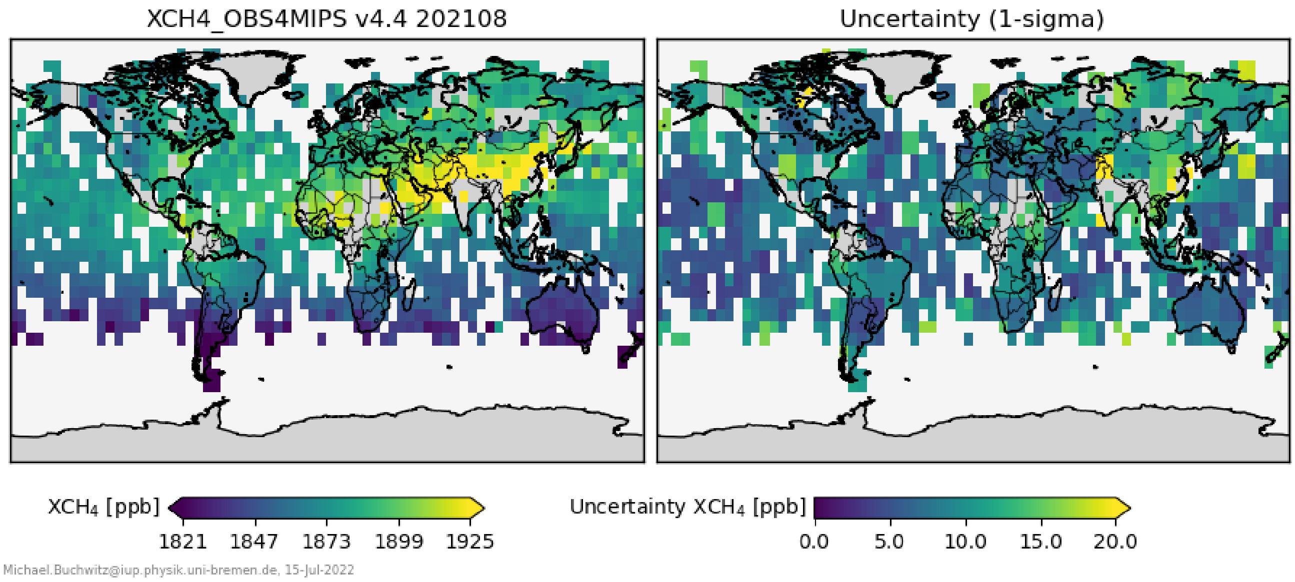


Figure 30 – OBS4MIPS XCH_4 (left) and corresponding uncertainty (right) for August 2021.



3.1.1 Obs4MIPS XCO_2 product format

The main quantity / data field is the column-average dry-air mole fraction of atmospheric carbon dioxide (CO_2), denoted XCO_2, as retrieved from the two satellite instruments SCIAMACHY/ENVISAT (Burrows et al., 1995; Bovensmann et al., 1999), TANSO-FTS/GOSAT (Kuze et al., 2009) and OCO-2 (Crisp et al., 2004; Boesch et al., 2011).

XCO_2 is a dimensionless quantity (unit: mol/mol) defined as the vertical column of CO_2 divided by the vertical column of dry air (= all air molecules except water vapor) (see, e.g., Buchwitz et al., 2005, for details). For example, if XCO_2 is 0.0004 (i.e., 400 ppm, parts per million) at a given location this means that there are 400 CO_2 molecules above that location per 1 million air molecules (excluding water vapour molecules).

Table 10 lists the main characteristics of this data product. See also Reuter et al., 2020, for an overview of why and how these products have been generated and for additional details.

The entire product is contained in a single file using this file name convention:

xco2_c3s_l3_v44_200301_202112.nc

Explanation:

- *xco2*: Variable name
- *c3s*: Copernicus Climate Change Service
- *l3*: Level 3 product
- *v44*: Version 4.4
- *200301_202112:* First month and last month of data set

Table 10: Main characteristics of the XCO_2 Obs4MIPs v4.4 product.

CF variable name, units	Long name: column-average dry-air mole fraction of atmospheric carbon dioxide Standard name: dry_atmosphere_mole_fraction_of_carbon_dioxide Units: dimensionless (mol/mol) See also: CF Standard Name Table, Version 31, 08 March 2016 (http://cfconventions.org/Data/cf-standard-names/31/build/cf-standard-name-table.html)
Spatial resolution	5° equal angle
Temporal resolution	Monthly average, from January 2003 – December 2021
Coverage	Global (2003 – mid 2009: land only; afterwards land and ocean)

Note that a resolution of 5^ox5^o has been selected (instead of, e.g., 1^ox1^o) to ensure better noise suppression (note that the underlying individual satellite retrievals are noisy and sparse due to very strict quality filtering) (see ATBD *D8*).

The variables as contained in the XCO_2 Obs4MIPs product file are listed in Table 11.

Table 11: XCO_2 Obs4MIPs v4.4 product variables.

Variable name	Short Description
xco2	Satellite retrieved column-average dry-air mole fraction of atmospheric carbon dioxide (CO_2) (Note: typical values are << 1.0 (typically close to 0.0004) and 1.0E20 = no data)
xco2_nobs	Number of individual XCO_2 Level 2 observation (per 5°x5° grid cell) used to compute the reported Level 3 XCO_2 monthly average value (0 = no data)
xco2_stderr	Reported uncertainty defined as standard error of the average including single sounding noise and potential seasonal and regional biases
xco2_stddev	Average standard deviation of the underlying XCO_2 Level 2 observations
time	Time in days since 1-Jan-1990
time_bnds	Time boundaries. Start and end time of each month in days since 1-Jan-1990
lat	Center latitude in degrees north (-90.0 to +90.0)
lat_bnds	Latitude boundaries (upper and lower boundaries of 5 deg latitude bands)
lon	Center longitude in degrees east (-180.0 to +180.0)
lon_bnds	Longitude boundaries (upper and lower boundaries of 5 deg longitude bands)
land_fraction	Fraction of 5 deg x 5 deg cells covered by land (numerical values are between 0.0 and 1.0)
pre	Pressure levels (dimensionsless as normalized to surface pressure)
pre_bnds	Pressure layer boundaries (dimensionsless as normalized to surface pressure)
column_averaging_kernel	XCO_2 averaging kernel (dimensionless); a vertical profile (1.0E20 = no data)
vmr_profile_co2_apriori	CO_2 volume mixing ratio profile (dimensionless fraction between 0.0 and 1.0; 1.0E20 = no data)

3.1.2 Obs4MIPS XCH_4 product format

The main quantity / data field is the column-average dry-air mole fraction of atmospheric methane (CH_4), denoted XCH_4, as retrieved from the two satellite instruments SCIAMACHY/ENVISAT (Burrows et al., 1995; Bovensmann et al., 1999) and TANSO-FTS/GOSAT (Kuze et al., 2009).

XCH_4 is a dimensionless quantity (unit: mol/mol) defined as the vertical column of CH_4 divided by the vertical column of dry air (= all air molecules except water vapor) (see, e.g., *Buchwitz et al., 2005*, for details). For example, if XCH_4 is 0.0000018 (i.e., 1800 ppb, parts per billion) at a given location this means that there are 1800 CH_4 molecules above that location per 1 billion air molecules (excluding water vapour molecules).

Table 12 lists the main characteristics of this data product. See also Reuter et al., 2020, for an overview and additional details.

The entire product is contained in a single file using this file name convention:

xch4_c3s_l3_v44_200301_202112.nc

Explanation:

- *xch4*: Variable name
- *c3s*: Copernicus Climate Change Service
- *l3*: Level 3 product
- *v44*: Version 4.4
- *200301_202112:* First month and last month of data set

Table 12: Main characteristics of the XCH4 Obs4MIPs v4.4 product.

CF variable name, units	Long name: column-average dry-air mole fraction of atmospheric methane Standard name: dry_atmosphere_mole_fraction_of_methane Units: dimensionless (mol/mol) See also: CF Standard Name Table, Version 31, 08 March 2016 (http://cfconventions.org/Data/cf-standard-names/31/build/cf-standard-name-table.html)
Spatial resolution	5° equal angle
Temporal resolution	Monthly average, from January 2003 – December 2021
Coverage	Global (November 2005 – March 2009: land only; before and afterwards land and ocean)

Note that a resolution of $5^o x 5^o$ has been selected (instead of, e.g., $1^o x 1^o$) to ensure better noise suppression (note that the underlying individual satellite retrievals are noisy and sparse due to very strict quality filtering).

The variables as contained in the XCH_4 Obs4MIPs product file are listed in Table 13.

Table 13: XCH_4 Obs4MIPs v4.4 product variables.

Variable name	Short Description
xch4	Satellite retrieved column-average dry-air mole fraction of atmospheric methane (CH_4) (Note: typical values are << 1.0 (typically close to 0.0000018) and 1.0E20 = no data)
xch4_nobs	Number of individual XCH_4 Level 2 observation (per 5°x5° grid cell) used to compute the reported Level 3 XCH_4 monthly average value (0 = no data)
xch4_stderr	Reported uncertainty defined as standard error of the average including single sounding noise and potential seasonal and regional biases
xch4_stddev	Average standard deviation of the underlying XCH_4 Level 2 observations
time	Time in days since 1-Jan-1990
time_bnds	Time boundaries. Start and end time of each month in days since 1-Jan-1990
lat	Center latitude in degrees north (-90.0 to +90.0)
lat_bnds	Latitude boundaries (upper and lower boundaries of 5 deg latitude bands)
lon	Center longitude in degrees east (-180.0 to +180.0)
lon_bnds	Longitude boundaries (upper and lower boundaries of 5 deg longitude bands)
land_fraction	Fraction of 5 deg x 5 deg cells covered by land (numerical values are between 0.0 and 1.0)
pre	Pressure levels (dimensionsless as normalized to surface pressure)
pre_bnds	Pressure layer boundaries (dimensionsless as normalized to surface pressure)
column_averaging_kernel	XCH_4 averaging kernel (dimensionless); a vertical profile (1.0E20 = no data)
vmr_profile_ch4_apriori	CH_4 volume mixing ratio profile (dimensionless fraction between 0.0 and 1.0; 1.0E20 = no data)

3.2 Target requirements

For a general overview on target requirements including Level 2 products please see Sect. 2.2.1. Here we address requirements and achieved performance of the Level 3 products.

The XCO_2 and XCH_4 products in Obs4MIPS format as presented in this section are Level 3 products with monthly time and 5°x5° spatial resolution.

Explicit requirements for Level 3 products are not formulated in *D7*. The development of satellite-derived gridded ECV products in Obs4MIPs format started in the framework ESA's Climate Change Initiative (CCI) via the GHG-CCI project[6] (see also Reuter et al., 2020). The envisaged main application is comparison with climate models. The GHG-CCI project team therefore proposed already several years ago to generate XCO_2 and XCH_4 products in Obs4MIPS format at the described spatio-temporal resolution. That spatio-temporal resolution was assumed to be appropriate for climate model comparisons taking into account also the characteristics of existing satellites. It was later confirmed by scientific studies (e.g., Lauer et al., 2017, and Gier et al., 2020) that the generated products were in fact very useful for the envisaged application.

As explicit target requirements for these products do not exist, it is assumed for the purpose of this project that the required accuracy (in terms of spatio-temporal biases) and stability (in terms of linear bias drift) is essentially identical with the corresponding requirement as listed in Table 8 for the Level 2 data products. With this assumption the achieved quality can be compared with the required quality and the findings can be summarized as follows (concerning the reported probabilities please see the more detailed discussion as presented in Sect. 2.2):

XCO_2 Level 3 product (see D9):

Figure 31 shows a comparison of Level 3 product XCO2_OBS4MIPS with TCCON XCO_2. Based on these and related assessments (see *D9*) the validation of Level 3 product XCO2_OBS4MIPS can be summarized as follows: The overall monthly mean uncertainty is 1.1 ppm and the mean bias is 0.28 ppm. Relative systematic errors, i.e., spatial and temporal biases amount to 0.5±0.6 ppm. The computed linear drift of 0.09±0.23 ppm is small and not significant. The probability that the 0.5 ppm accuracy requirement is met is 68%. The probability that the 0.5 ppm/year stability requirement is met is 95%. Overall, this product has therefore reasonable accuracy and high stability.

XCH_4 Level 3 product (see D9):

Figure 32 shows a comparison of Level 3 product XCH4_OBS4MIPS with TCCON XCH_4. Based on these and related assessments (see *D9*) the validation of Level 3 product XCH4_OBS4MIPS can be summarized as follows: The overall monthly mean uncertainty is 7.9 ppb and the mean bias is 4.4 ppb. Relative systematic errors, i.e., spatial and temporal biases amount to 4.7±6 ppb. The computed linear drift of 0.45±1.2 ppb is small and not significant. The probability that the 10 ppb

[6] https://climate.esa.int/en/projects/ghgs/ (last access: 5-Apr-2023)

accuracy requirement is met is 89%. The probability that the 3 ppb/year stability requirement is met is 98%. Overall, this product has therefore very good accuracy and high stability.

Figure 31 - Overview data quality assessment results for Level 3 XCO_2 Obs4MIPs format data product. Note that each dot corresponds to a given TCCON site and month.

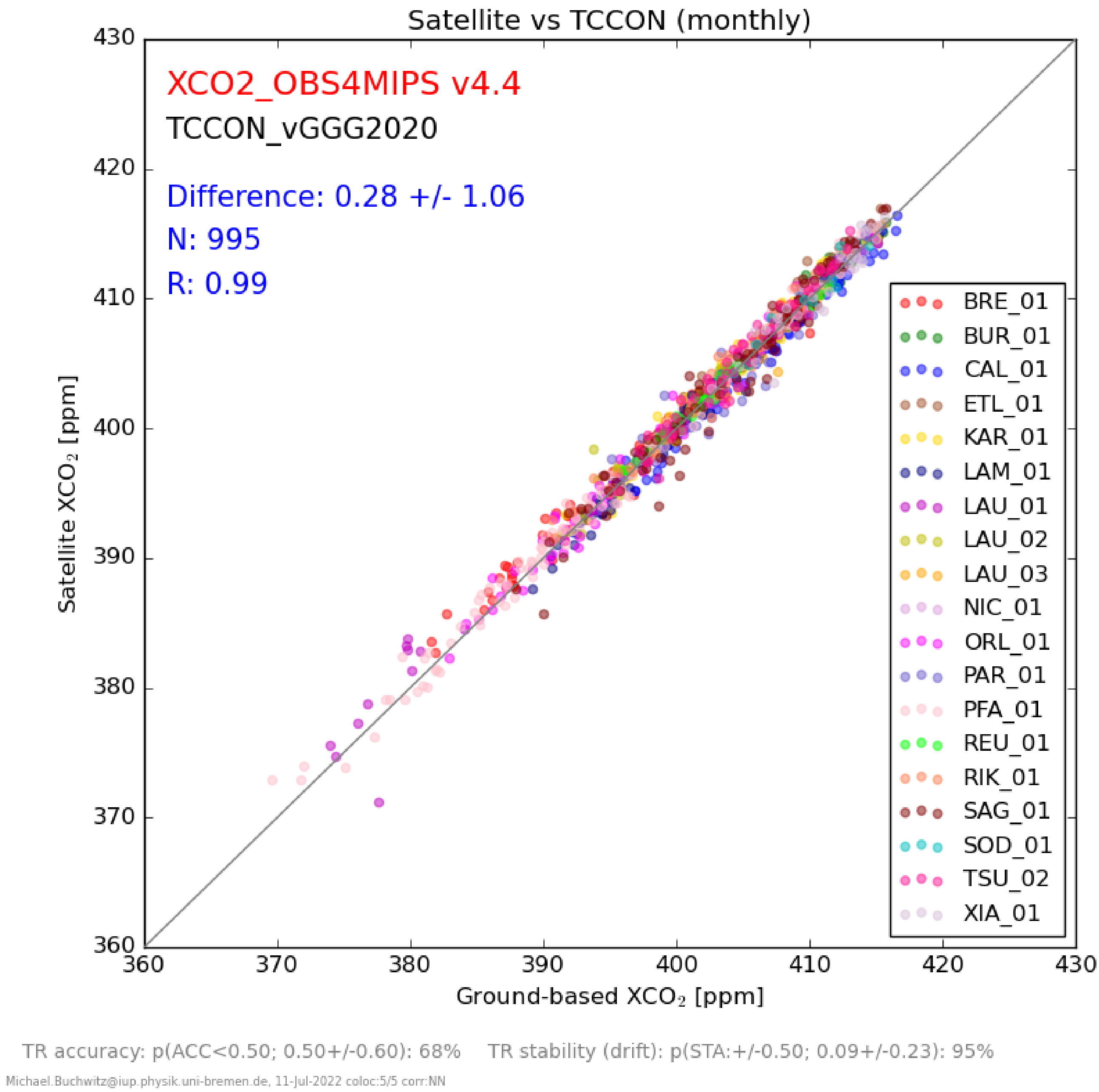
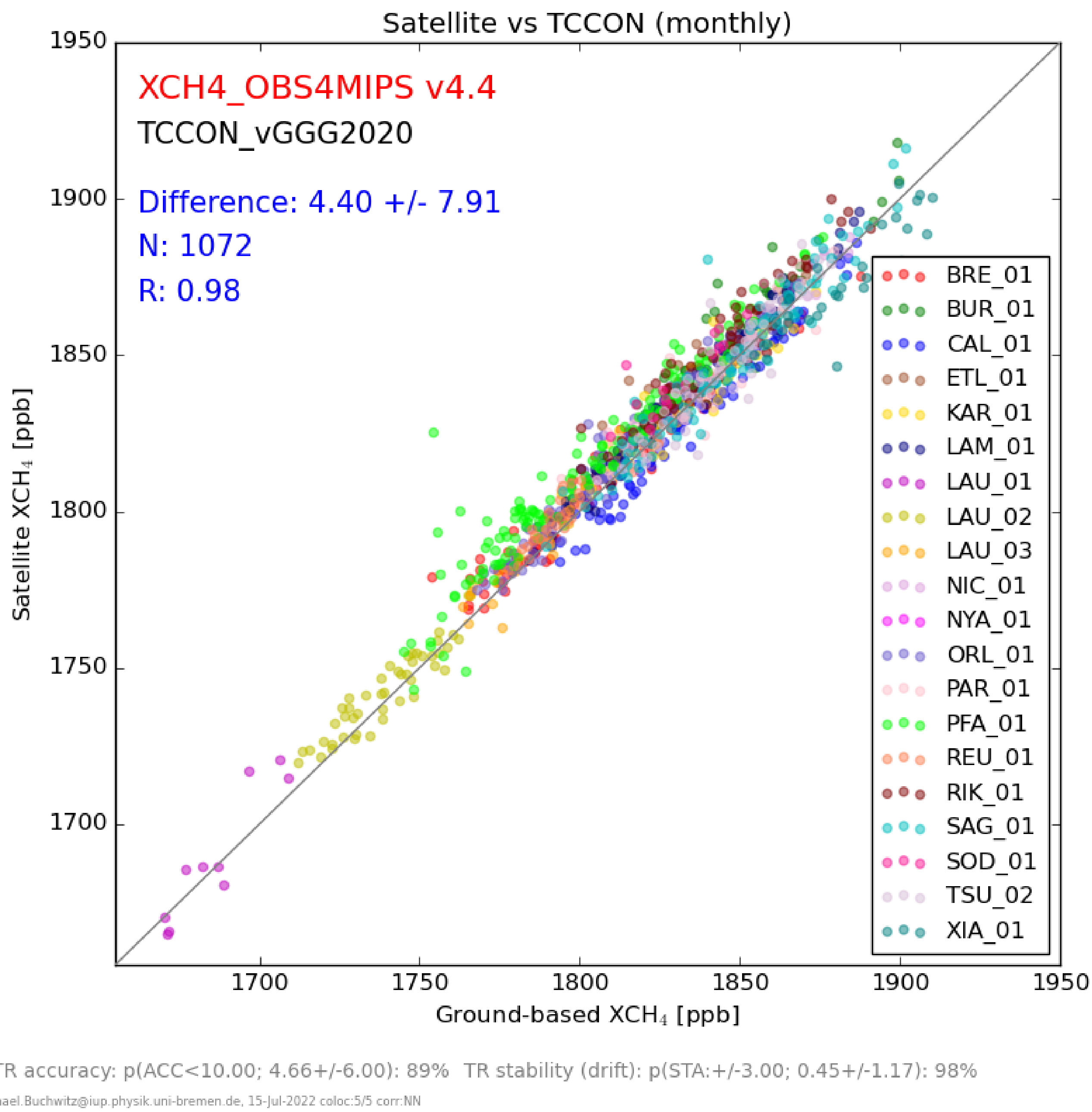


Figure 32 - Overview data quality assessment results for Level 3 XCH_4 Obs4MIPs format data product. Note that each dot corresponds to a given TCCON site and month.



3.3 Data usage information

The data format is described in detail in Sect. 3.1.1 for XCO_2 and in Sect. 3.1.2 for XCH_4. As shown in these sections, the main variables of these Level 3 products are xco2 and xch4, the column-averaged dry-air mole fractions of XCO_2 and XCH_4, respectively. In contrast to the corresponding Level 2 products, the units used here are not ppm (10^{-6}) or ppb (10^{-9}) but are dimensionless quantities in mol/mol, i.e., they are reported as numerical fractional values in the range 0.0 – 1.0.

Also reported (in the same units) are the corresponding (1-sigma) uncertainties (variables xco2_stderr and xch4_stderr). These variables are reported per month and per 5^ox5^o (latitude times longitude) grid cell. Also provided are variables related to spatial (variables lat, lat_bnds, lon, lon_bnds) and temporal information (time, time_bnds) as described in detail in Sects. 3.1.1 and 3.1.2. How these products "look like" is shown in several figures in this document (Figure 27 - Figure 30).

Similar to the Level 2 products (see Sect. 2.1) information on altitude sensitivity (variable column_averaging_kernel) and *a priori* profiles (variables vmr_profile_co2_apriori and vmr_profile_ch4_apriori) is also provided.

The Level 3 Obs4MIPs XCO_2 and XCH_4 products have been primarily generated for comparison with climate models, see, for example Lauer et al., 2017, and Gier et al., 2020, but have also been used for other applications such as computations of annual mean atmospheric growth rates (e.g., Buchwitz et al., 2018; Reuter et al., 2020).

The Level 3 XCO_2 and XCH_4 v4.4 Obs4MIPS format data products described in this document (in combination with more recent satellite XCO_2 and XCH_4 retrievals from the CAMS project[7]) have been used for the Copernicus Press Release from January 2023: "Copernicus: 2022 was a year of climate extremes, with record high temperatures and rising concentrations of greenhouse gases"[8].

The products do not have any known issues.

[7] https://atmosphere.copernicus.eu (last access: 5-Apr-2023)

[8] https://climate.copernicus.eu/copernicus-2022-was-year-climate-extremes-record-high-temperatures-and-rising-concentrations (last access: 5-Apr-2023)

4. Level 2 mid-tropospheric CO_2 and CH_4 data products

4.1 Product description

These products contain the IASI mid-tropospheric CO_2 and CH_4 mixing ratios and the AIRS mid-tropospheric CO_2 mixing ratio, i.e., the description given in this section is valid for these products:

- CO2_IASA_NLIS (product from IASI on Metop-A)
- CO2_IASB_NLIS (product from IASI on Metop-B)
- CH4_IASA_NLIS (product from IASI on Metop-A)
- CH4_IASB_NLIS (product from IASI on Metop-B)
- CO2_AIRS_NLIS (product from AIRS; as generated in a pre-cursor project; not updated in this project)

The format of these products is essentially identical as the Level 2 XCO_2 and XCH_4 data product format described in Sect. 2.

They only exceptions are:

- xco2 needs to be replaced by co2 (e.g., co2_quality_flag instead of xco2_quality_flag)
- xch4 needs to be replaced by ch4 (e.g., ch4_quality_flag instead of xch4_quality_flag)
- All other variable names are the same but note that some contain -999.0 for "no valid data" (e.g., some angles and uncertainty).

For additional details see the corresponding PUGS ANNEX E (see Sect. 7.5).

4.2 Target requirements

For a general overview on target requirements including Level 2 XCO_2 and XCH_4 products please see Sect. 2.2.1. Here we address requirements and achieved performance of the Level 2 mid-tropospheric products.

As explained in Sect. 2.2, we use existing instruments to generate Level 2 products and, therefore, spatio-temporal resolution and sampling are determined by satellite instrument and satellite characteristics and a comparison of achieved performance with required performance does not make sense. Instead, we report here the relevant spatio-temporal characteristics:

- IASI instruments on Metop satellites:
  - Spatial resolution 12 km at nadir
  - Swath width 2200 km
  - Global coverage twice a day

The TRDGAD (*D7*) document contains requirements for the CO_2 and CH_4 mid-tropospheric data products for random errors, systematic errors and stability in terms of goal (G), breakthrough (B) and threshold (T) requirements. The numerical values of these requirements are identical with the numerical values as listed in Table 8, i.e., the requirements as listed in Table 8 are also applicable for the CO_2 and CH_4 mid-tropospheric data products.

Detailed assessment results related to the quality of these data products are provided in document *D9* and can be summarized as follows:

Summary quality IASI CO_2 products (see D9):

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

Summary quality IASI CH_4 products (see D9):

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

Comparison of required performance with achieved performance:

As an overall summary, Table 14 presents and overview of the required performance for random and systematic error and stability with the achieved performance for the Level 2 CO_2 and CH_4 mid-tropospheric data products as generated in this project.

Table 14: Comparison of required performance (see *D7*) with achieved performance in terms of probability that the corresponding requirement is met (see *D6*). Listed are only products as generated in this project. (*) Not assessed, e.g., due to lack of reference data. (#) Achieved performance in mixing ratio units in brackets.

	Random error single observation	**Systematic error (spatio-temporal bias)**	**Stability (linear bias drift)**	**Comment**
	Level 2 mid-tropospheric CO_2 products:			
Required (T)	**< 8 ppm (#)**	**< 0.5 ppm**	**< 0.5 ppm/year**	
Achieved:	Probability that threshold requirement is met:			
CO2_IASA_NLIS	100% (1 ppm)	50%	100%	
CO2_IASB_NLIS	100% (1 ppm)	(*)	(*)	
	Level 2 mid-tropospheric CH_4 products:			
Required (T)	**< 34 ppb (#)**	**< 10 ppb**	**< 3 ppb/year**	
Achieved:	Probability that threshold requirement is met:			
CH4_IASA_NLIS	100% (12 ppb)	90%	(*)	
CH4_IASB_NLIS	100% (12 ppb)	(*)	(*)	

4.3 Data usage information

The data format is described in detail in Sect. 2.1.

As explained in that section, the main variables are co2 (in ppm) and ch4 (in ppb). Also reported are the corresponding (1-sigma) uncertainties (variables co2_uncertainty (in ppm) and ch4_uncertainty (in ppb)). Important is also the quality flag (variables co2_quality_flag and ch4_quality_flag). For "good" data the numerical value of the quality flag is 0 (zero). All results shown in this document (and in other documents such as *D9* presenting the validation and comparison results) are for "good" data with quality flag = 0. All Level 2 product contain this variable but some only contain "good" data. It is strongly recommended to use this variable and to use only data with quality flag = 0.

These variables are reported per satellite footprint along with spatial (variables latitude and longitude) and temporal information (variable time). The latitudes and longitudes are the footprint centre coordinates. This information is provided for all Level 2 data products (see common variables in Sect. 2.1.1). The individual satellite data products may contain additional information such as footprint corner coordinates (see the product specific Annexes to this main PUGS document as listed in Sect. 7). Furthermore, for each footprint additional information is provided such as averaging kernels (variables co2_averaging_kernel and ch4_averaging_kernel) and corresponding pressure levels (variable pressure_levels) (see Sect. 2.1).

The data products have been used to study atmospheric trends and variability, for comparison with models and to obtain information on sources and sinks as shown in a number of publications such as Chevallier et al., 2005, 2009a; Crevoisier et al., 2004, 2009, 2009b, 2013; Cressot et al., 2014.

The products do not have any known issues.

5. Data access information

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

Direct link to CO_2 products:
https://cds.climate.copernicus.eu/cdsapp#!/dataset/satellite-carbon-dioxide?tab=overview

Direct link to CH_4 products:
https://cds.climate.copernicus.eu/cdsapp#!/dataset/satellite-methane?tab=overview

Tabs / riders lead to the following items:

- Overview
    - Short overview of all products
- Download data
    - Data access information
- Quality assessment
    - The CDS datasets are assessed by the Evaluation and Quality Control (EQC) function of C3S independently of the data supplier and the EQC information are available on this site.
- Documentation
    - Links to the following documents:
        - Algorithm Theoretical Basis Document (ATBD)
        - Product User Guide (PUG)
        - Product Quality Assurance Document (PQAD)
        - Product Quality Assessment Report (PQAR)
        - System Quality Assurance Document (SQAD)
        - Target Requirements and Gap Analysis (TRDGAD)
    - Note that pdf versions of all documents (including previous versions) are (also) available from here: https://www.iup.uni-bremen.de/carbon_ghg/cg_data.html#C3S_GHG
- View
    - Visualization of selected data products in terms of global maps

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

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

7. List of ANNEXes

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

7.1 ANNEX A: PUGS for products CO2_GOS_OCFP, CH4_GOS_OCFP and CH4_OCPR

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

7.2 ANNEX B: PUGS for products CO2_GO2_SRFP and CH4_GO2_SRFP

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

7.3 ANNEX C: PUGS for product CH4_GO2_SRPR

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

7.4 ANNEX D: PUGS for XCO2_EMMA, XCH4_EMMA, XCO2_OBS4MPIS, XCH4_OBS4MIPS

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

7.5 ANNEX E: PUGS for IASI CO_2 and CH_4 and AIRS CO_2 mid-tropospheric products

Describes the mid-tropospheric CO_2 and CH_4 products from the IASI instrument series generated by LMD/CNRS, France. Also describes the AIRS mid-tropospheric CO_2 product as generated in a pre-cursor project.

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

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

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

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