



# Product User Guide and Specification (PUGS) – ANNEX D for products XCO2\_EMMA, XCH4\_EMMA, XCO2\_OBS4MIPS, XCH4\_OBS4MIPS (v4.4, 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 (2003-2016)	All
2.0	4-October-2018	Update for CDR2 (2003-2017)	All
3.0	12-August-2019	Update for CDR3 (2003-2018)	All
3.1	03-November-2019	Update after review by Assimila: Correction of typos. Figure captions moved to above figures.	All
4.0	18-August-2020	Update for CDR4 (2003-2019)	All
5.0	18-February-2021	Update for CDR5 (01/2003-06/2020)	All
6.0	4-August-2022	Update for CDR6 (01/2003-12/2021)	All
6.1	6-December-2022	Update after review (use of new template, several improvements at various places)	All
6.3	18-April-2023	Update after 2 <sup>nd</sup> review. 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	XCO2_EMMA, XCH4_EMMA, XCO2_OBS4MIPS, XCH4_OBS4MIPS	CDR 6	4.4	31-Aug-2022

## Related documents

Reference ID	Document
D1	<p>Main PUGS:</p> <p><b>Buchwitz, M., et al., 2023:</b> Product User Guide and Specification (PUGS) – Main document for Greenhouse Gas (GHG: CO<sub>2</sub> &amp; CH<sub>4</sub>) data set CDR 6 (2003-2021), project C3S2_312a_Lot2_DLR – Atmosphere, v6.3, 2023.</p> <p><i>(This document is an ANNEX to the Main PUGS)</i></p>
D2	<p>Corresponding ATBD:</p> <p><b>ATBD ANNEX D:</b> Reuter, M., et al., Algorithm Theoretical Basis Document (ATBD) – ANNEX D for products XCO2_EMMA, XCH4_EMMA, XCO2_OBS4MIPS, XCH4_OBS4MIPS (v4.4, 01/2003-12/2021), project C3S2_312a_Lot2_DLR – Atmosphere, v6.2, 2023.</p>
D3	<p><b>TRD GAD GHG, 2020:</b> Buchwitz, M., Aben, I., Armante, R., Boesch, H., Crevoisier, C., Hasekamp, O. P., Wu, L., Reuter, M., Schneising-Weigel, O., Target Requirement and Gap Analysis Document, Copernicus Climate Change Service (C3S) project on satellite-derived Essential Climate Variable (ECV) Greenhouse Gases (CO<sub>2</sub> and CH<sub>4</sub>) data products (project C3S_312b_Lot2), Version 2.11, 9-April-2020, pp. 80, 2020.</p>



## 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 <i>neuronal</i> network mid/upper tropospheric CO <sub>2</sub> and CH <sub>4</sub> 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 Wave InfraRed
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 InfraRed
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<sub>2</sub>) 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 a Product User Guide and Specification (PUGS) for the Copernicus Climate Change Service (C3S, <https://climate.copernicus.eu/>) greenhouse gas (GHG) component as covered by project C3S2\_312a\_Lot2.

Within this project satellite-derived atmospheric carbon dioxide (CO<sub>2</sub>) and methane (CH<sub>4</sub>) Essential Climate Variable (ECV) data products are being generated and delivered to ECMWF for inclusion into the Copernicus Climate Data Store (CDS) from which users can access these data products and the corresponding documentation.

The satellite-derived GHG data products are:

- Column-averaged dry-air mixing ratios (mole fractions) of CO<sub>2</sub> and CH<sub>4</sub>, denoted XCO<sub>2</sub> (in parts per million, ppm) and XCH<sub>4</sub> (in parts per billion, ppb), respectively.
- Mid/upper tropospheric mixing ratios of CO<sub>2</sub> (in ppm) and CH<sub>4</sub> (in ppb).

This document describes the version 4.4 C3S products XCO<sub>2</sub>\_EMMA, XCH<sub>4</sub>\_EMMA, XCO<sub>2</sub>\_OBS4MIPS, and XCH<sub>4</sub>\_OBS4MIPS.

These products are merged multi-sensor XCO<sub>2</sub> and XCH<sub>4</sub> level 2 and level 3 products generated using algorithms developed at the University of Bremen, Germany (see D1, D2 and Reuter et al. (2013, 2020)).



## Executive summary

The EMMA database consists of individual level 2 soundings retrieved by algorithms which can change from grid box to grid box and month to month. It can be used in the same manner as any other XCO<sub>2</sub> or XCH<sub>4</sub> satellite retrieval, i.e., the EMMA database includes all information needed for inverse modeling (geo-location, time, XCO<sub>2</sub> or XCH<sub>4</sub>, averaging kernels, etc.).

The data fields and guidance on their use are provided in the main PUGS document (D1) describing, e.g., the common variables of all XCO<sub>2</sub> and XCH<sub>4</sub> L2 data sets provided by the Copernicus project C3S2\_312a\_Lot2.

Additionally, to the common variables, EMMA includes information on, e.g., the inter-algorithm spread which informs about potential regional uncertainties and on the source-algorithm of each individual sounding within the EMMA data base. Such variables are the subject of this ANNEX describing the EMMA v4.4 CO<sub>2</sub> and EMMA v4.4 CH<sub>4</sub> specific aspects of the EMMA L2 data base.

The L3 data products XCO<sub>2</sub>\_OBS4MIPS and XCH<sub>4</sub>\_OBS4MIPS are generated by spatial (5°x5°) and temporal (monthly) gridding of the corresponding EMMA L2 data bases. Additional information to what can be found in this document about the data format, content, and user guidelines can be obtained from the main PUGS document (D1).

The following sections describe the products XCO<sub>2</sub>\_EMMA (v4.4) (Section 1), XCO<sub>2</sub>\_EMMA (v4.4) (Section 2), XCO<sub>2</sub>\_EMMA (v4.4) (Section 3), and XCO<sub>2</sub>\_EMMA (v4.4) (Section 4). Section 5 provides information on how to access the data.



## 1. Product XCO<sub>2</sub>\_EMMA (v4.4)

### 1.1 Product description

The XCO<sub>2</sub>\_EMMA data product is a Level 2 XCO<sub>2</sub> data product in the same format as the other C2S2\_312a\_Lot2 project Level 2 XCO<sub>2</sub> data products (see main PUGS document (D1)), i.e., all common variables are also variables of this data product.

Additionally, to the common variables, the EMMA L2 data product includes the variables listed in Table 1 and described in the following.

Table 2 list all individual sensor / individual algorithm L2 products, which have been used as input for the generation of the EMMA XCO<sub>2</sub> L2 product.

**Table 1:** EMMA v4.4 XCO<sub>2</sub> product specific variables.

Name	Type	Dimension	Units	Short Description
median_processor_id	Integer	n	[-]	A unique ID for each L2 algorithm contributing to EMMA
median_uncertainty	Float	n	ppm, i.e., 10 <sup>-6</sup>	Inter algorithm spread defined as standard deviation of the L3 products in the corresponding grid box (see D2)
median_uncertainty_se	Float	n	ppm, i.e., 10 <sup>-6</sup>	Standard error of the median uncertainty (see D2)
median_uncertainty_ex	Float	n	ppm, i.e., 10 <sup>-6</sup>	Inter-algorithm spread as expected from measurement noise (see D2)
xco2_accuracy	Float	n	ppm, i.e., 10 <sup>-6</sup>	Potential spatio/temporal XCO <sub>2</sub> bias (1-sigma) estimated from TCCON co-locations (see D2)
contributing_algorithms	Byte	n	[-]	Number of L2 algorithms contributing to median calculation in a specific grid box



### Description of each parameter:

#### ***median\_processor\_id***

A unique ID for each L2 algorithm contributing to EMMA. See listing in Table 2.

#### ***median\_uncertainty***

Inter algorithm spread defined as standard deviation of the L3 products in the corresponding grid box (see D2).

#### ***median\_uncertainty\_se***

Standard error of the median uncertainty (see D2).

#### ***median\_uncertainty\_ex***

Inter-algorithm spread as expected from measurement noise (see D2).

#### ***xco2\_accuracy***

Potential spatio/temporal XCO<sub>2</sub> bias (1-sigma) estimated from TCCON co-locations (see D2).

#### ***contributing\_algorithms***

Number of L2 algorithms contributing to median calculation in a specific grid box.

**Table 2:** L2 algorithms used in EMMA v4.4 XCO<sub>2</sub>.

Satellite/Instrument	Algorithm	Institution	ID	Reference
SCIAMACHY	BESD v02.01.02	IUP	2	Reuter et al. (2010, 2011, 2016)
GOSAT	NIES v02.9xbc (bias corrected)	NIES	3	Yoshida et al. (2013)
GOSAT	RemoTeC v2.3.8	SRON	5	Butz et al. (2011), Detmers et al. (2017a)
GOSAT	UoL-FP v7.3	UoL	6	Cogan et al (2012) Boesch and Anand (2017)
GOSAT	ACOS v9r	NASA	7	O'Dell et al. (2012), Taylor et al. (2022)
GOSAT	FOCAL v3.0	IUP	8	Noël et al. (2022)
OCO-2	NASA v10.2	NASA	9	Kiel et al. (2019)
OCO-2	FOCAL v10	IUP	10	Reuter et al. (2017a,b, 2021)
GOSAT-2	RemoTeC v2.0.0	SRON	12	Krisna et al. (2021)
GOSAT-2	FOCAL v3.0	IUP	13	Noël et al. (2022)





## 1.2 Target requirements

The target requirements for these products are described in the Target Requirement Document (TRD) (see D3).

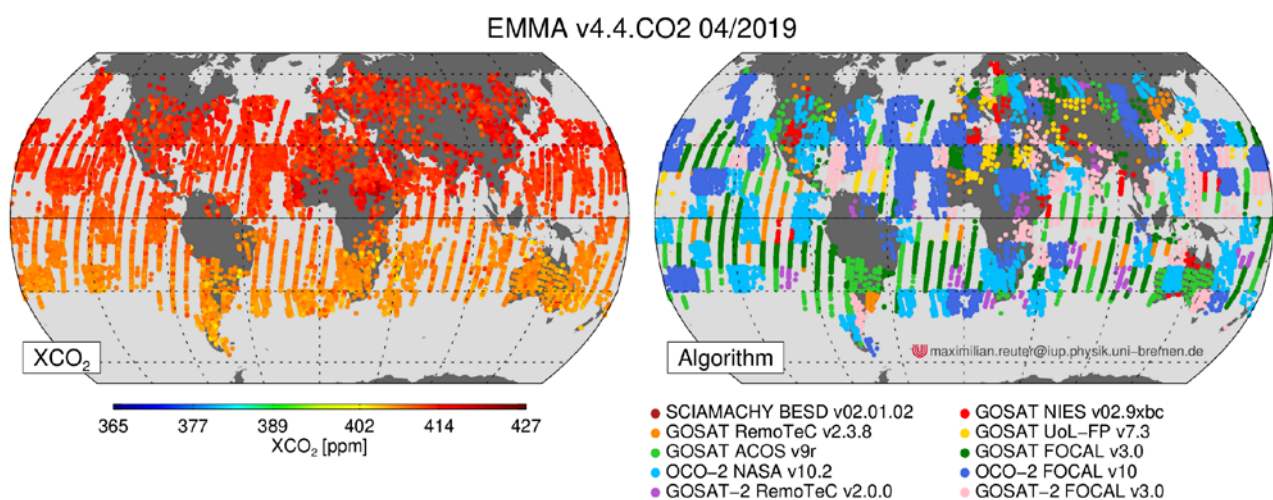
A summary of the assessment of the data quality including a comparison with the target requirements is given in the main PUGS document (see D1).

## 1.3 Data usage information

The EMMA data product consists of individual level 2 soundings which can be used in the same manner as any other XCO<sub>2</sub> satellite retrievals, i.e., the EMMA L2 data product includes all information needed for inverse modelling (geo-location, time, XCO<sub>2</sub>, averaging kernels, etc.). The main PUGS document (D1) provides guidance on how to use the information.

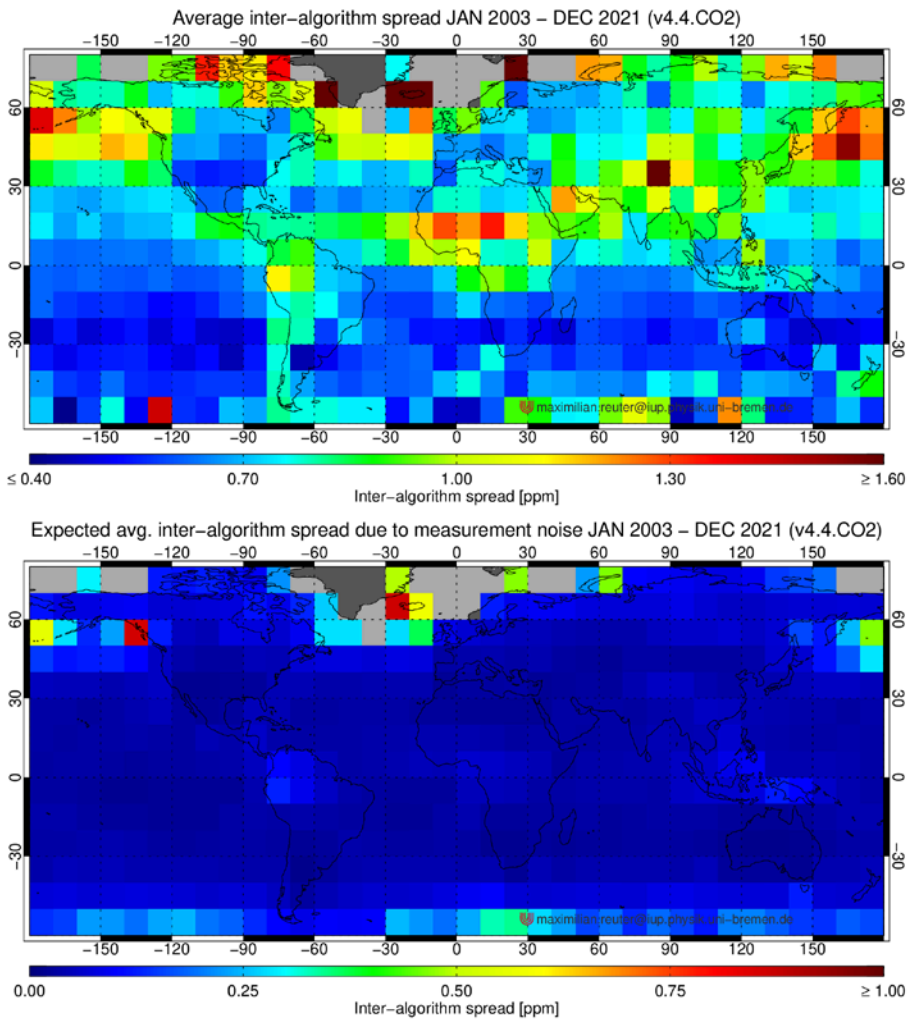
Figure 1 shows for an example month (April 2019) the EMMA XCO<sub>2</sub> and the corresponding algorithms selected by the EMMA algorithm (see D2). Figure 2 shows the average inter-algorithm spread and the expected average inter-algorithm spread due to measurement noise.

**Figure 1:** EMMA L2 XCO<sub>2</sub> (left) and corresponding selected algorithm (right) for EMMA v4.4 XCO<sub>2</sub> for April 2019.





**Figure 2: Average inter-algorithm spread (01/2003 – 12/2021) (top) and the expected average inter-algorithm spread due to measurement noise (bottom).**





## 2. Product XCH<sub>4</sub>\_EMMA (v4.4)

### 2.1 Product description

The XCH<sub>4</sub>\_EMMA data product is a Level 2 XCH<sub>4</sub> data product in the same format as the other C2S2\_312a\_Lot2 project Level 2 XCH<sub>4</sub> data products (see main PUGS document (D1)), i.e., all common variables are also variables of this data product.

Additionally, to the common variables, the EMMA L2 data product includes the variables listed in Table 3 and described in the following.

Table 4 lists all individual sensor / individual algorithm level 2 products, which have been used as input for the generation of the EMMA XCH<sub>4</sub> product.

**Table 3:** EMMA v4.4 XCH<sub>4</sub> product specific variables.

Name	Type	Dimension	Units	Short Description
median_processor_id	Integer	n	[-]	A unique ID for each L2 algorithm contributing to EMMA
median_uncertainty	Float	n	ppb, i.e., 10 <sup>-9</sup>	Inter algorithm spread defined as standard deviation of the L3 products in the corresponding grid box (see D2)
median_uncertainty_se	Float	n	ppb, i.e., 10 <sup>-9</sup>	Standard error of the median uncertainty (see D2)
median_uncertainty_ex	Float	n	ppb, i.e., 10 <sup>-9</sup>	Inter-algorithm spread as expected from measurement noise (see D2)
xch4_accuracy	Float	n	ppb, i.e., 10 <sup>-9</sup>	Potential spatio/temporal XCH <sub>4</sub> bias (1-sigma) estimated from TCCON co-locations (see D2)
contributing_algorithms	Byte	n	[-]	Number of L2 algorithms contributing to median calculation in a specific grid box



### Description of each parameter:

#### ***median\_processor\_id***

A unique ID for each L2 algorithm contributing to EMMA. See listing in Table 4.

#### ***median\_uncertainty***

Inter algorithm spread defined as standard deviation of the L3 products in the corresponding grid box (see D2).

#### ***median\_uncertainty\_se***

Standard error of the median uncertainty (see D2).

#### ***median\_uncertainty\_ex***

Inter-algorithm spread as expected from measurement noise (see D2).

#### ***xch4\_accuracy***

Potential spatio/temporal XCH<sub>4</sub> bias (1-sigma) estimated from TCCON co-locations (see D2).

#### ***contributing\_algorithms***

Number of L2 algorithms contributing to median calculation in a specific grid box.

**Table 4:** L2 algorithms used in EMMA v4.4 CH<sub>4</sub>.

Satellite/Instrument	Algorithm	Institution	ID	Reference
SCIAMACHY	WFMD v4.0	IUP	2	Schneising et al. (2018)
GOSAT	FOCAL-FP v3.0	IUP	3	Noël et al. (2022)
GOSAT	FOCAL-PR v3.0	IUP	4	Noël et al. (2022)
GOSAT	NIES v02.9xbc (bias corrected)	NIES	5	Yoshida et al. (2013)
GOSAT	RemoTeC-FP v2.3.8	SRON	7	Butz et al. (2011), Detmers et al. (2017a)
GOSAT	RemoTeC-PR v2.3.9	SRON	8	Butz et al. (2011), Detmers et al. (2017b)
GOSAT	UoL-FP v7.3	UoL	9	Cogan et al (2012) Boesch and Anand (2017)
GOSAT	UoL-PR v9.0	UoL	10	Cogan et al (2012) Boesch and Anand (2017)
GOSAT-2	FOCAL-FP v3.0	IUP	11	Noël et al. (2022)
GOSAT-2	FOCAL-PR v3.0	IUP	12	Noël et al. (2022)
GOSAT-2	RemoTeC-FP v2.0.0	SRON	13	Krisna et al. (2021)
GOSAT-2	RemoTeC-PR v2.0.0	SRON	14	Krisna et al. (2021)
GOSAT-2	NIES v01.07	NIES	15	Yoshida and Oshio (2020)



## 2.2 Target requirements

The target requirements for these products are described in the Target Requirement Document (TRD) (see D3).

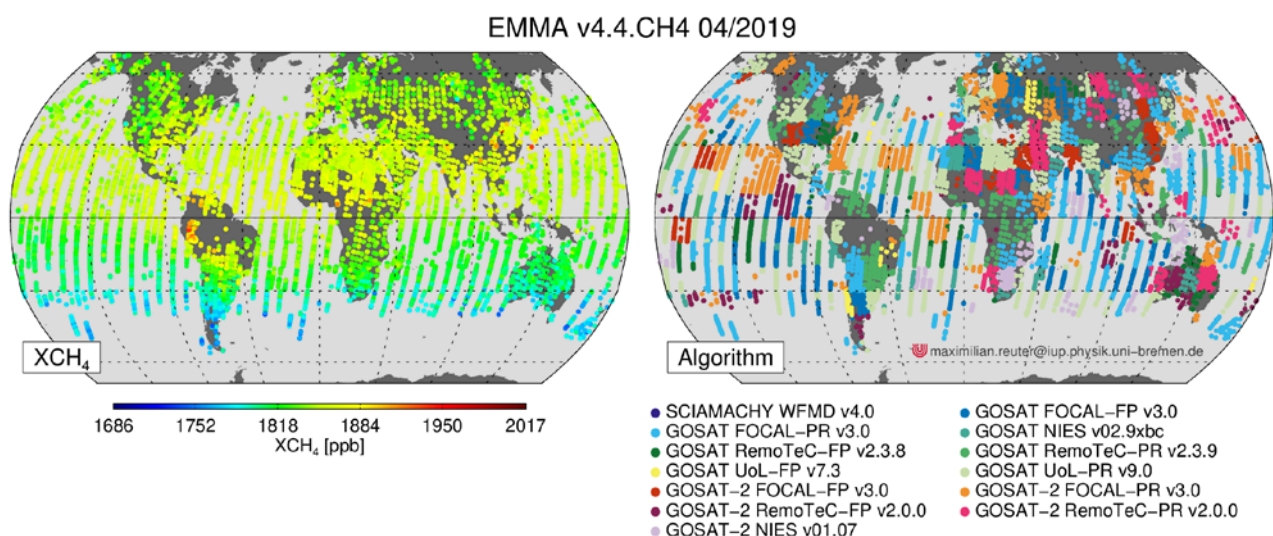
A summary of the assessment of the data quality including a comparison with the target requirements is given in the main PUGS document (see D1).

## 2.3 Data usage information

The EMMA data product consists of individual level 2 soundings which can be used in the same manner as any other XCH<sub>4</sub> satellite retrievals, i.e., the EMMA L2 data product includes all information needed for inverse modelling (geo-location, time, XCH<sub>4</sub>, averaging kernels, etc.). The main PUGS document (D1) provides guidance on how to use the information.

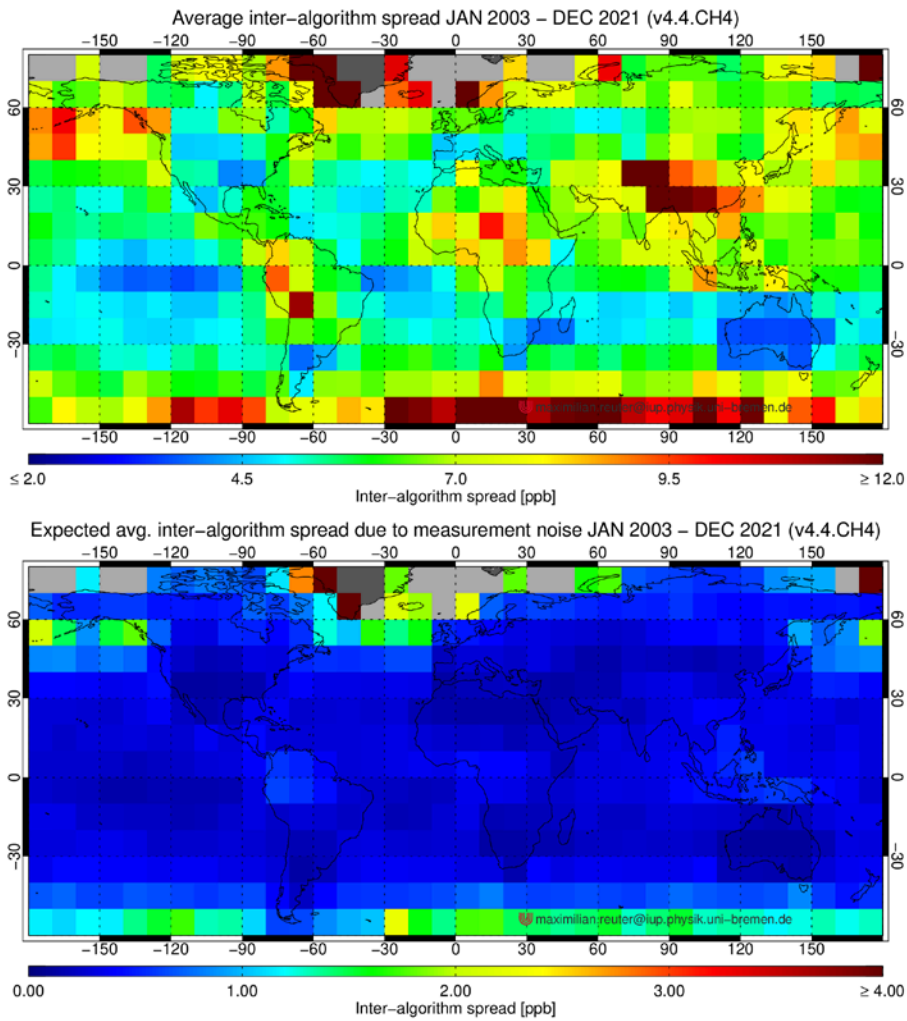
Figure 3 shows for an example month (April 2019) the EMMA XCH<sub>4</sub> and the corresponding algorithms selected by the EMMA algorithm (see D2). Figure 4 shows the average inter-algorithm spread and the expected average inter-algorithm spread due to measurement noise.

**Figure 3:** EMMA L2 XCH<sub>4</sub> (left) and corresponding selected algorithm (right) for EMMA v4.4 XCH<sub>4</sub> for April 2019.





**Figure 4:** Average inter-algorithm spread (01/2003 – 12/2021) (**top**) and the expected average inter-algorithm spread due to measurement noise (**bottom**).





### 3. Product XCO<sub>2</sub>\_OBS4MIPS (v4.4)

#### 3.1 Product description

Obs4MIPs (Observations for Model Intercomparisons Project) is an activity to make observational products more accessible especially for climate model intercomparisons.

The XCH<sub>4</sub>\_OBS4MIPS data product is in Obs4MIPs NetCDF format, which is described on the Obs4MIPs website<sup>1</sup>.

The XCH<sub>4</sub>\_OBS4MIPS product is generated by spatial (5°x5°) and temporal (monthly) gridding of the corresponding EMMA L2 product. The OBS4MIPS L3 XCH<sub>4</sub> product includes the variables listed in Table 5. They are described in the following.

**Table 5:** XCO<sub>2</sub>\_OBS4MIPS variables. x, y, z, t, represent the number of grid points in longitude, latitude, pressure, and temporal dimension respectively.

Name	Type	Dimension	Units	Short Description
time	Float	t	Days since 1990-01-01	Time center
time_bnds	Float	t,2	Days since 1990-01-01	Time boundaries
lat	Float	y	Degrees north	Latitude center
lat_bnds	Float	y,2	Degrees north	Latitude boundaries
lon	Float	x	Degrees east	Longitude center
lon_bnds	Float	x,2	Degrees east	Longitude boundaries
pre	Float	z	Surface pressure	Pressure center
pre_bnds	Float	z,2	Surface pressure	Pressure boundaries
land_fraction	Float	x,y	1	Land area fraction
xco2	Float	x,y,t	1	Satellite retrieved column-average dry-air mole fraction of CO <sub>2</sub>
xco2_nobs	Integer	x,y,t	1	Number of individual L2 observations
xco2_stddev	Float	x,y,t	1	Standard error
xco2_stddev	Float	x,y,t	1	Standard deviation
column averaging kernel	Float	x,y,z,t	1	Column-averaging kernel

<sup>1</sup> <https://pcmdi.github.io/obs4MIPs/> (last access: 27.01.2023)



vmr_profile_co2_apriori	Float	x,y,z,t	1	A priori dry-air mole fraction profile
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**Description of each parameter:**

***time, time\_bnds***

Time center and boundaries in days since 1990-01-01.

***lat, lat\_bnds***

Latitude center and boundaries in degrees north.

***lon, lon\_bnds***

Longitude center and boundaries in degrees east.

***pre, pre\_bnds***

Pressure center and boundaries in units of surface pressure.

***land\_fraction***

Land area fraction computed from GTOPO30 data available from the U.S. Geological Survey.

***xco2***

Main parameter: satellite retrieved column-average dry-air mole fraction of CO<sub>2</sub>.

***xco2\_nobs***

Number of individual L2 observations per grid box.

***xco2\_stddev***

Standard error of the average computed from the single sounding noise and potential seasonal and regional biases, i.e., the inter algorithm spread.

***xco2\_stddev***

Standard deviation of the L2 observations within each grid box.

***column averaging kernel***

The normalized column-averaging kernel represents the sensitivity of the retrieved XCO<sub>2</sub> to the true mole fraction depending on pressure (height). All values represent layer averages within the corresponding pressure levels. Values near one are ideal and indicate that the influence of the a priori is minimal. Profiles are ordered from surface to top of atmosphere.

***vmr\_profile\_co2\_apriori***

A priori dry-air mole fraction profile of atmospheric CO<sub>2</sub>. All values represent layer averages within the corresponding pressure levels. Profiles are ordered from surface to top of atmosphere. The a priori profile is needed to apply the column averaging kernel.





### 3.2 Target requirements

The target requirements for these products are described in the Target Requirement Document (TRD) (see D3).

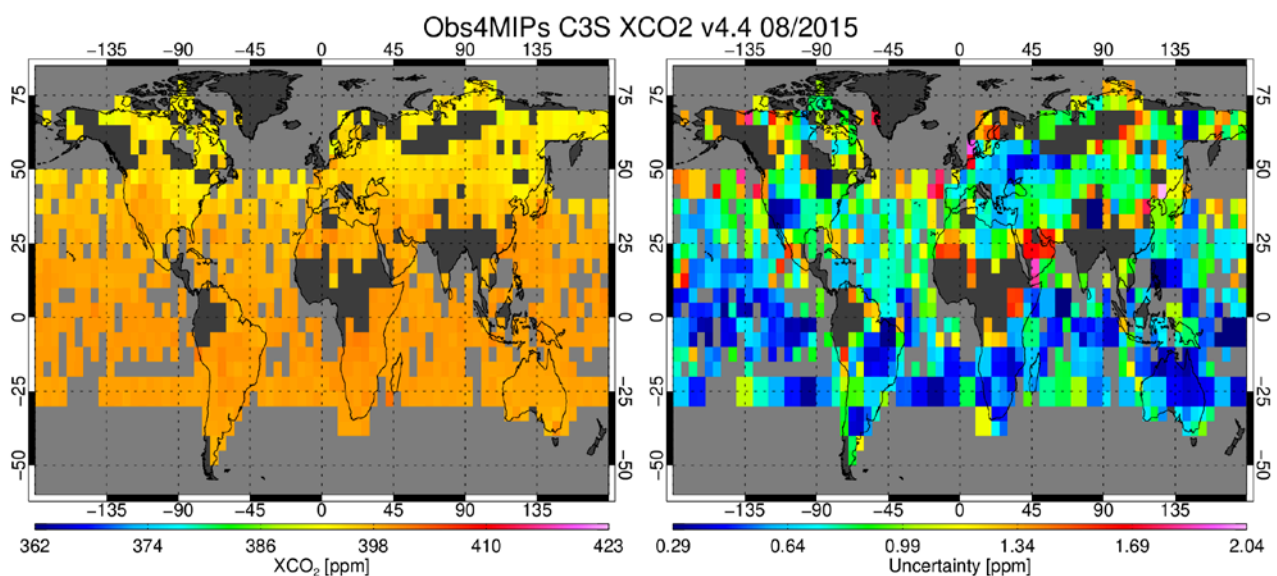
A summary of the assessment of the data quality including a comparison with the target requirements is given in the main PUGS document (see D1).

### 3.3 Data usage information

The XCO<sub>2</sub>\_OBS4MIPS and XCH<sub>4</sub>\_OBS4MIPS products consist of spatially (5°x5°) and temporal (monthly) gridded EMMA L2 data. Among other parameters, the data files include averaged XCO<sub>2</sub> satellite retrievals and uncertainties, column averaging kernels, and a priori profiles. The main PUGS document (D1) provides guidance on how to use this information.

Figure 5 shows for an example month (August 2015) the OBS4MIPS XCO<sub>2</sub> and the corresponding uncertainty computed from the retrieval noise and EMMA’s inter-algorithm spread (see D2).

**Figure 5:** XCO<sub>2</sub>\_OBS4MIPS XCO<sub>2</sub> for August 2015 (**left**) and its uncertainty computed from the retrieval noise and EMMA’s inter-algorithm spread (**right**).





## 4. Product XCH4\_OBS4MIPS (v4.4)

### 4.1 Product description

Obs4MIPs (Observations for Model Intercomparisons Project) is an activity to make observational products more accessible especially for climate model intercomparisons. The XCH4\_OBS4MIPS data product is in Obs4MIPs NetCDF format, which is described on the Obs4MIPs website<sup>2</sup>. The XCH4\_OBS4MIPS product is generated by spatial (5°x5°) and temporal (monthly) gridding of the corresponding EMMA L2 product. The OBS4MIPS L3 XCH<sub>4</sub> product include the variables listed in Table 6. They are described in the following.

**Table 6:** XCH4\_OBS4MIPS variables. x, y, z, t, represent the number of grid points in longitude, latitude, pressure, and temporal dimension respectively.

Name	Type	Dimension	Units	Short Description
time	Float	t	Days since 1990-01-01	Time center
time_bnds	Float	t,2	Days since 1990-01-01	Time boundaries
lat	Float	y	Degrees north	Latitude center
lat_bnds	Float	y,2	Degrees north	Latitude boundaries
lon	Float	x	Degrees east	Longitude center
lon_bnds	Float	x,2	Degrees east	Longitude boundaries
pre	Float	z	Surface pressure	Pressure center
pre_bnds	Float	z,2	Surface pressure	Pressure boundaries
land_fraction	Float	x,y	1	Land area fraction
xch4	Float	x,y,t	1	Satellite retrieved column-average dry-air mole fraction of CH <sub>4</sub>
xch4_nobs	Integer	x,y,t	1	Number of individual L2 observations
xch4_stdder	Float	x,y,t	1	Standard error
xch4_stddev	Float	x,y,t	1	Standard deviation
column averaging kernel	Float	x,y,z,t	1	Column-averaging kernel
vmr_profile_ch4_apriori	Float	x,y,z,t	1	A priori dry-air mole fraction profile

<sup>2</sup> <https://pcmdi.github.io/obs4MIPs/> (last access: 27.01.2023)

**Description of each parameter:*****time, time\_bnds***

Time center and boundaries in days since 1990-01-01.

***lat, lat\_bnds***

Latitude center and boundaries in degrees north.

***lon, lon\_bnds***

Longitude center and boundaries in degrees east.

***pre, pre\_bnds***

Pressure center and boundaries in units of surface pressure.

***land\_fraction***

Land area fraction computed from GTOPO30 data available from the U.S. Geological Survey.

***xch4***

Main parameter: satellite retrieved column-average dry-air mole fraction of CH<sub>4</sub>.

***xch4\_nobs***

Number of individual L2 observations per grid box.

***xch4\_stddev***

Standard error of the average computed from the single sounding noise and potential seasonal and regional biases, i.e., the inter algorithm spread.

***xch4\_stddev***

Standard deviation of the L2 observations within each grid box.

***column averaging kernel***

The normalized column-averaging kernel represents the sensitivity of the retrieved XCH<sub>4</sub> to the true mole fraction depending on pressure (height). All values represent layer averages within the corresponding pressure levels. Values near one are ideal and indicate that the influence of the a priori is minimal. Profiles are ordered from surface to top of atmosphere.

***vmr\_profile\_ch4\_apriori***

A priori dry-air mole fraction profile of atmospheric CH<sub>4</sub>. All values represent layer averages within the corresponding pressure levels. Profiles are ordered from surface to top of atmosphere. The a priori profile is needed to apply the column averaging kernel.



## 4.2 Target requirements

The target requirements for these products are described in the Target Requirement Document (TRD) (see D3).

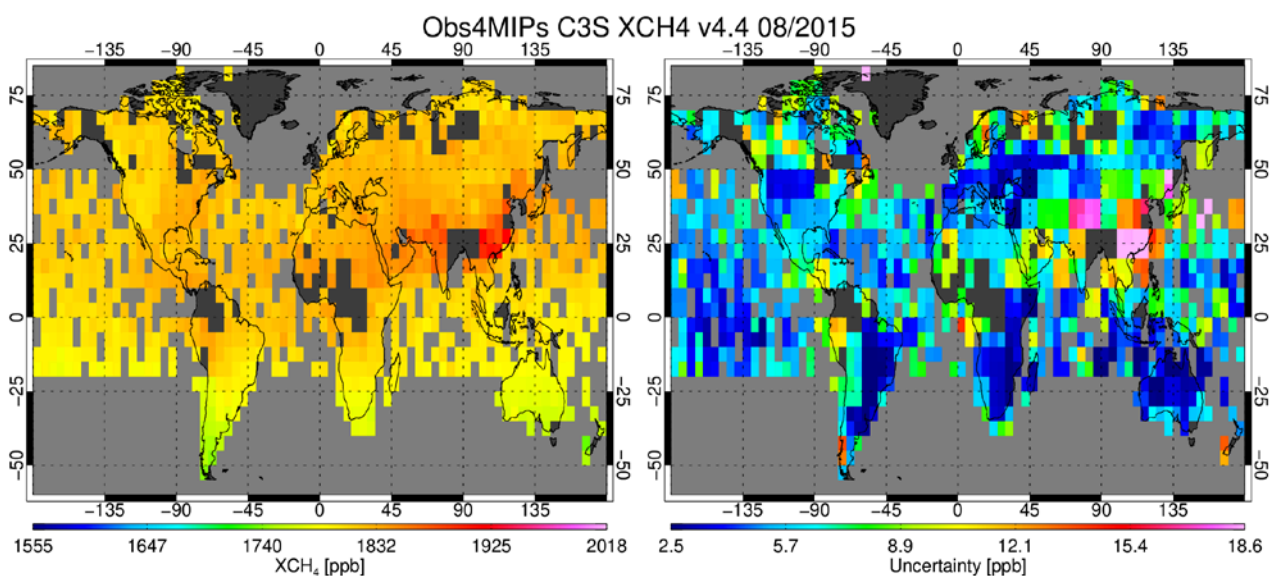
A summary of the assessment of the data quality including a comparison with the target requirements is given in the main PUGS document (see D1).

## 4.3 Data usage information

The XCO<sub>2</sub>\_OBS4MIPS and XCH<sub>4</sub>\_OBS4MIPS products consist of spatially (5°x5°) and temporal (monthly) gridded EMMA L2 data. Among other parameters, the data files include averaged XCO<sub>2</sub> or XCH<sub>4</sub> satellite retrievals and uncertainties, column averaging kernels, and a priori profiles. The main PUGS document (D1) provides guidance on how to use this information.

Figure 6 shows for an example month (August 2015) the OBS4MIPS XCO<sub>2</sub> and XCH<sub>4</sub> and the corresponding uncertainty computed from the retrieval noise and EMMA’s inter-algorithm spread (see D2).

**Figure 6:** XCH<sub>4</sub>\_OBS4MIPS XCH<sub>4</sub> for August 2015 (left) and its uncertainty computed from the retrieval noise and EMMA’s inter-algorithm spread (right).





## 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<sub>2</sub> products including documentation:

<https://cds.climate.copernicus.eu/cdsapp#!/dataset/satellite-carbon-dioxide?tab=overview>

Direct link to CH<sub>4</sub> products including documentation:

<https://cds.climate.copernicus.eu/cdsapp#!/dataset/satellite-methane?tab=overview>

Tabs / riders lead to the following items:

- Overview
  - Short overview of all products
  - Licence
  - Contact
- 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](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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