

ECMWF COPERNICUS REPORT

Copernicus Climate Change Service



# Product User Guide and Specification (PUGS) – ANNEX D for products XCO2\_EMMA, XCH4\_EMMA, XCO2\_OBS4MIPS, XCH4\_OBS4MIPS (v4.5, 01/2003-12/2022)

# 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
7.0	24-August-2023	Update for data set CDR7 (temporal coverage: 2003-2022)	All
7.2	13-November-2023	Minor improvements after review	All

## List of datasets covered by this document

Deliverable ID	Product title	Product type (CDR, ICDR)	Version number	Delivery date
WP2-FDDP-GHG-v2	XCO2_EMMA, XCH4_EMMA, XCO2_OBS4MIPS, XCH4_OBS4MIPS	CDR 7	4.5	31-Aug-2023

### **Related documents**

Reference ID	Document
D1	Main PUGS: <b>Buchwitz, et al., 2023:</b> Product User Guide and Specification (PUGS) – Main document for Greenhouse Gas (GHG: CO <sub>2</sub> & CH <sub>4</sub> ) data set CDR 7 (2003-2022), project C3S2_312a_Lot2_DLR – Atmosphere, 2023.
	(This document is an ANNEX to the Main PUGS)
D2	Corresponding ATBD: <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 (v4.5, 01/2003-12/2022), project C3S2_312a_Lot2_DLR – Atmosphere, 2023.
D3	<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.



### 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		
ССІ	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		

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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)			
ОСО	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	
ТВС	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, <u>https://climate.copernicus.eu/</u>) 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 v4.5 C3S products XCO2\_EMMA, XCH4\_EMMA, XCO2\_OBS4MIPS, and XCH4\_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 v4.5 CO<sub>2</sub> and EMMA v4.5 CH<sub>4</sub> specific aspects of the EMMA L2 data base.

The L3 data products XCO2\_OBS4MIPS and XCH4\_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 XCO2\_EMMA (v4.5) (Section 1), XCO2\_EMMA (v4.5) (Section 2), XCO2\_EMMA (v4.5) (Section 3), and XCO2\_EMMA (v4.5) (Section 4). Section 5 provides information on how to access the data.



### 1. Product XCO2\_EMMA (v4.5)

### **1.1 Product description**

The XCO2\_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  $XCO_2$  L2 product.

Name	Туре	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_s e	Float	n	ppm, i.e., 10 <sup>-6</sup>	Standard error of the median uncertainty (see D2)
median_uncertainty_e x	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_algorith ms	Byte	n	[-]	Number of L2 algorithms contributing to median calculation in a specific grid box

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



### 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.



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 v11.1	NASA	9	Kiel et al. (2019)
OCO-2	FOCAL v10.1	IUP	10	Reuter et al. (2017a,b, 2021)
GOSAT-2	NIES v02.00	NIES	11	Yoshida and Oshio (2020)
GOSAT-2	RemoTeC v2.0.0	SRON	12	Krisna et al. (2021)
GOSAT-2	FOCAL v3.0	IUP	13	Noël et al. (2022)

### Table 2: L2 algorithms used in EMMA v4.5 XCO<sub>2</sub>.

### **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).

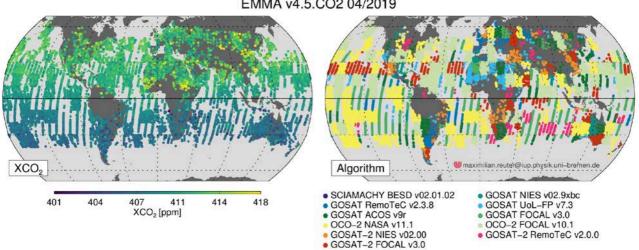


### 1.3 Data usage information

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 v4.5 XCO<sub>2</sub> for April 2019.



EMMA v4.5.CO2 04/2019

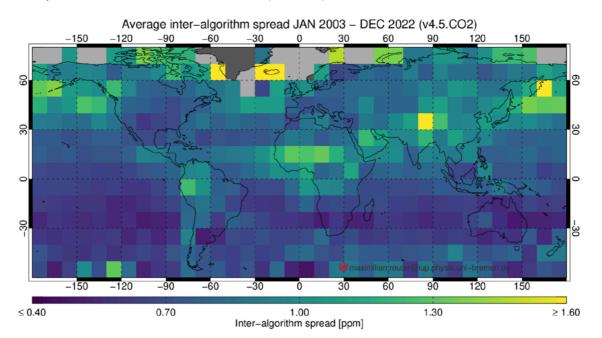
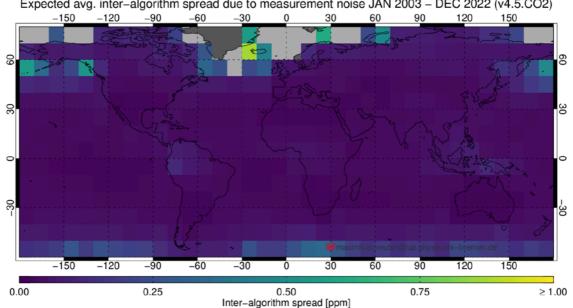


Figure 2: Average inter-algorithm spread (01/2003 – 12/2022) (top) and the expected average interalgorithm spread due to measurement noise (bottom).



Expected avg. inter-algorithm spread due to measurement noise JAN 2003 - DEC 2022 (v4.5.CO2)



### 2. Product XCH4\_EMMA (v4.5)

### **2.1 Product description**

The XCH4\_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.

Name	Туре	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_s e	Float	n	ppb, i.e., 10 <sup>-9</sup>	Standard error of the median uncertainty (see D2)
median_uncertainty_e x	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 XCH4 bias (1-sigma) estimated from TCCON co-locations (see D2)
contributing_algorith ms	Byte	n	[-]	Number of L2 algorithms contributing to median calculation in a specific grid box

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



### 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.



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 v2.0.1	SRON	14	Krisna et al. (2021)
GOSAT-2	NIES v02.00	NIES	15	Yoshida and Oshio (2020)

### Table 4: L2 algorithms used in EMMA v4.5 CH<sub>4</sub>.

### 2.2 Target requirements

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

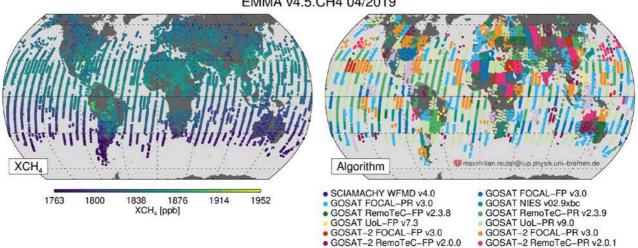
A summary of the assessment of the data quality including a comparison with the target requirements is given in the main PUGS document (see D1).

### 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 v4.5 XCH<sub>4</sub> for April 2019.



EMMA v4.5.CH4 04/2019

GOSAT-2 RemoTeC-FP v2.0.0 GOSAT-2 NIES v02.00

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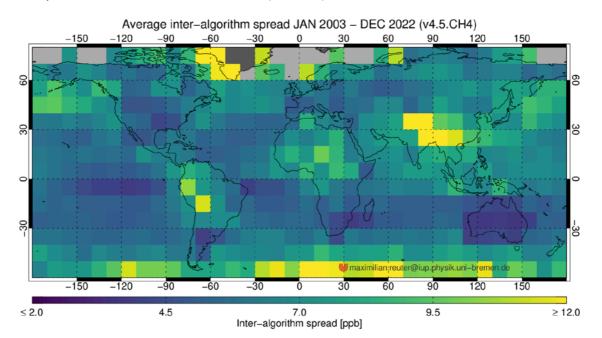
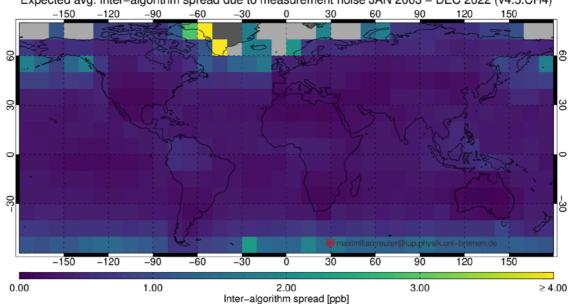


Figure 4: Average inter-algorithm spread (01/2003 – 12/2022) (top) and the expected average interalgorithm spread due to measurement noise (bottom).



Expected avg. inter-algorithm spread due to measurement noise JAN 2003 - DEC 2022 (v4.5.CH4)



### 3. Product XCO2\_OBS4MIPS (v4.5)

### **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 XCH4\_OBS4MIPS data product is in Obs4MIPs NetCDF format, which is described on the Obs4MIPs website<sup>1</sup>.

The XCH4\_OBS4MIPS product is generated by spatial ( $5^{\circ}x5^{\circ}$ ) 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:** XCO2\_OBS4MIPS variables. x, y, z, t, represent the number of grid points in longitude, latitude, pressure, and temporal dimension respectively.

Name	Туре	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	У	Degrees north	Latitude center
lat_bnds	Float	у,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	х,у	1	Land area fraction
хсо2	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_stdder	Float	x,y,t	1	Standard error
xco2_stddev	Float	x,y,t	1	Standard deviation

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

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column averaging kernel	Float	x,y,z,t	1	Column-averaging kernel
vmr_profile_co2_ap riori	Float	x,y,z,t	1	A priori dry-air mole fraction profile

### 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.

#### хсо2

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\_stdder

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).

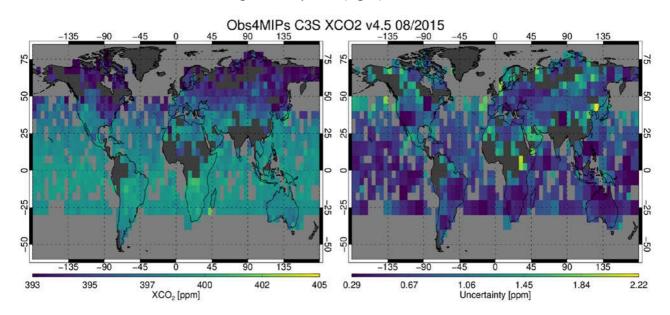
A summary of the assessment of the data quality including a comparison with the target requirements is given in the main PUGS document (see D1).

### 3.3 Data usage information

The XCO2\_OBS4MIPS and XCH4\_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:** XCO2\_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 (v4.5)

### 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.

Name	Туре	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	у	Degrees north	Latitude center
lat_bnds	Float	у,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	х,у	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

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

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



vmr_profile_ch4_apriori	Float	x,y,z,t	1	A priori dry-air mole
				fraction profile

### **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\_stdder

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.

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### 4.2 Target requirements

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

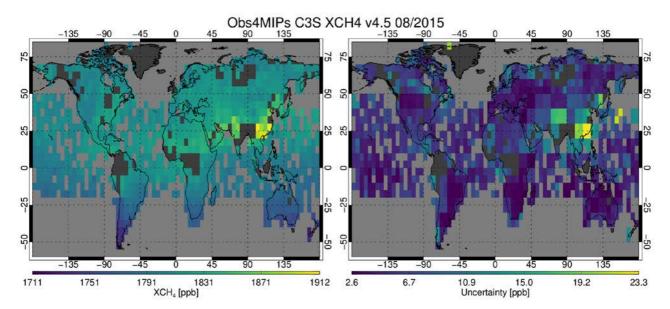
A summary of the assessment of the data quality including a comparison with the target requirements is given in the main PUGS document (see D1).

### 4.3 Data usage information

The XCO2\_OBS4MIPS and XCH4\_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:** XCH4\_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
  - o Short overview of all products
  - o Licence
  - o 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: <u>https://www.iup.uni-bremen.de/carbon\_ghg/cg\_data.html#C3S\_</u>GHG
- View
  - Visualization of selected data products in terms of global maps

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