

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 nd 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: Buchwitz, et al., 2023: Product User Guide and Specification (PUGS) – Main document for Greenhouse Gas (GHG: CO ₂ & CH ₄) 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: ATBD ANNEX D: 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	TRD GAD GHG, 2020: Buchwitz, M., Aben, I., Armante, R., Boesch, H., Crevoisier, C., Hasekamp, O. P., Wu, L., Reuter, M., Schneising-Weigel, O., Target Requirement and Gap Analysis Document, Copernicus Climate Change Service (C3S) project on satellite-derived Essential Climate Variable (ECV) Greenhouse Gases (CO ₂ and CH ₄) data products (project C3S_312b_Lot2), Version 2.11, 9-April-2020, pp. 80, 2020.



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 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)			
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., XCO₂) 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 (CO₂) and methane (CH₄) 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 CO₂ and CH₄, denoted XCO₂ (in parts per million, ppm) and XCH₄ (in parts per billion, ppb), respectively.
- Mid/upper tropospheric mixing ratios of CO₂ (in ppm) and CH₄ (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 XCO₂ and XCH₄ 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 XCO₂ or XCH₄ satellite retrieval, i.e., the EMMA database includes all information needed for inverse modeling (geo-location, time, XCO₂ or XCH₄, 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 XCO₂ and XCH₄ 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 CO₂ and EMMA v4.5 CH₄ 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 XCO₂ data product in the same format as the other C2S2_312a_Lot2 project Level 2 XCO₂ 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 ⁻⁶	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 ⁻⁶	Standard error of the median uncertainty (see D2)
median_uncertainty_e x	Float	n	ppm, i.e., 10 ⁻⁶	Inter-algorithm spread as expected from measurement noise (see D2)
xco2_accuracy	Float	n	ppm, i.e., 10 ⁻⁶	Potential spatio/temporal XCO ₂ 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 XCO₂ 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 XCO₂ 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 XCO₂.

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).

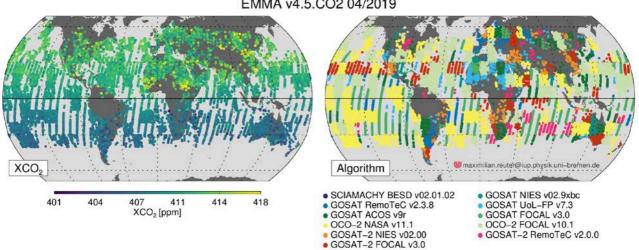


1.3 Data usage information

The EMMA data product consists of individual level 2 soundings which can be used in the same manner as any other XCO₂ satellite retrievals, i.e., the EMMA L2 data product includes all information needed for inverse modelling (geo-location, time, XCO₂, 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 XCO₂ 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 XCO₂ (left) and corresponding selected algorithm (right) for EMMA v4.5 XCO₂ for April 2019.



EMMA v4.5.CO2 04/2019

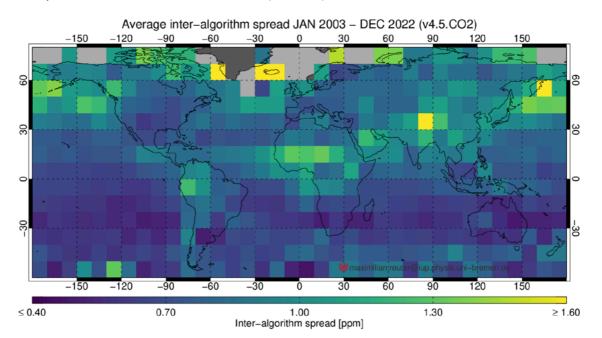
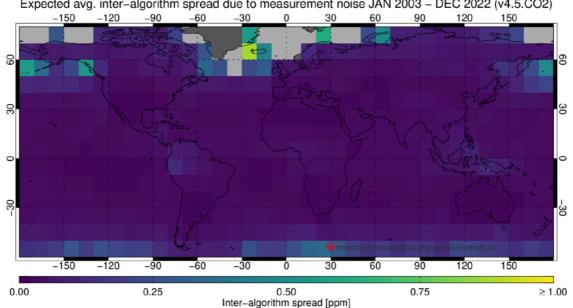


Figure 2: Average inter-algorithm spread (01/2003 – 12/2022) (top) and the expected average interalgorithm spread due to measurement noise (bottom).



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 XCH₄ data product in the same format as the other C2S2_312a_Lot2 project Level 2 XCH₄ 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 XCH₄ 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 ⁻⁹	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 ⁻⁹	Standard error of the median uncertainty (see D2)
median_uncertainty_e x	Float	n	ppb, i.e., 10 ⁻⁹	Inter-algorithm spread as expected from measurement noise (see D2)
xch4_accuracy	Float	n	ppb, i.e., 10 ⁻⁹	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 XCH₄ 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 XCH₄ 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 CH₄.

2.2 Target requirements

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

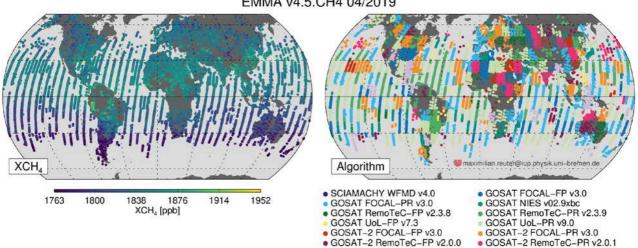
A summary of the assessment of the data quality including a comparison with the target requirements is given in the main PUGS document (see D1).

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 XCH₄ satellite retrievals, i.e., the EMMA L2 data product includes all information needed for inverse modelling (geo-location, time, XCH₄, 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 XCH₄ 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 XCH₄ (left) and corresponding selected algorithm (right) for EMMA v4.5 XCH₄ 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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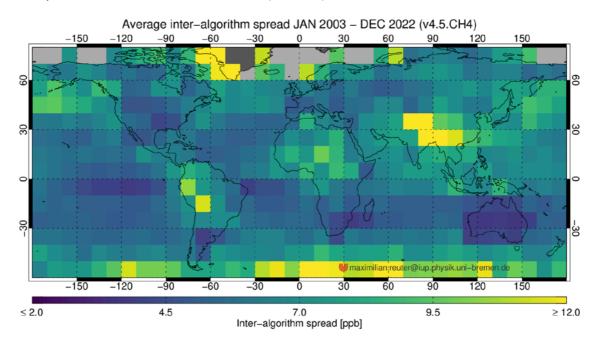
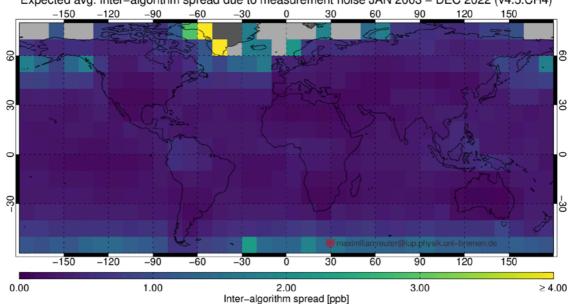


Figure 4: Average inter-algorithm spread (01/2003 – 12/2022) (top) and the expected average interalgorithm spread due to measurement noise (bottom).



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 website¹.

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 XCH₄ 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 ₂
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

¹ <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 CO₂.

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 XCO₂ 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 CO₂. 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).

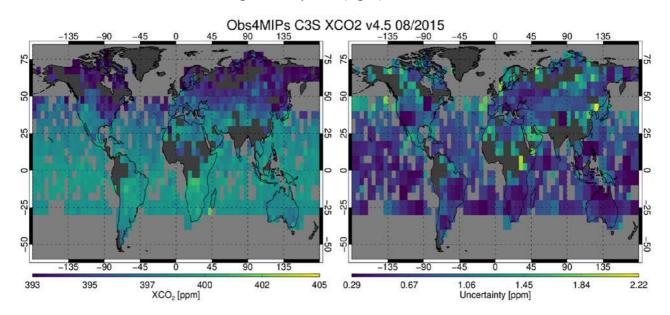
A summary of the assessment of the data quality including a comparison with the target requirements is given in the main PUGS document (see D1).

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 XCO₂ 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 XCO₂ and the corresponding uncertainty computed from the retrieval noise and EMMA's inter-algorithm spread (see D2).

Figure 5: XCO2_OBS4MIPS XCO₂ 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 website². The XCH4_OBS4MIPS product is generated by spatial (5°x5°) and temporal (monthly) gridding of the corresponding EMMA L2 product. The OBS4MIPS L3 XCH₄ 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 ₄
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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² <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 CH₄.

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 XCH₄ 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 CH₄. 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).

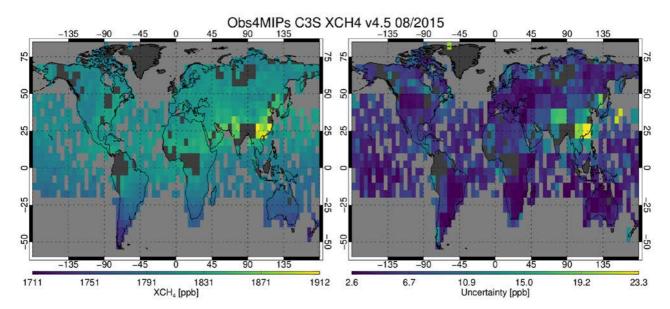
A summary of the assessment of the data quality including a comparison with the target requirements is given in the main PUGS document (see D1).

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 XCO₂ or XCH₄ 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 XCO₂ and XCH₄ and the corresponding uncertainty computed from the retrieval noise and EMMA's inter-algorithm spread (see D2).

Figure 6: XCH4_OBS4MIPS XCH₄ 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 CO₂ products including documentation:

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

Direct link to CH₄ 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

References

Boesch and Anand, 2017: H. Boesch and J. Anand, Algorithm Theoretical Basis Document (ATBD) – ANNEX A for products CO2_GOS_OCFP, CH4_GOS_OCFP & CH4_GOS_OCPR, Copernicus Climate Change Service (C3S) project on satellite-derived Essential Climate Variable (ECV) Greenhouse Gases (CO₂ and CH₄) data products (project C3S_312a_Lot6), Version 1 (21/08/2017), 2017.

Buchwitz, et al., 2023: Product User Guide and Specification (PUGS) – Main document for Greenhouse Gas (GHG: CO₂ & CH₄) data set CDR 7 (2003-2022), project C3S2_312a_Lot2_DLR – Atmosphere, v7.0, 2023.

Butz et al., 2011: Butz, A., Guerlet, S., Hasekamp, O., Schepers, D., Galli, A.,Aben, I., Frankenberg, C., Hartmann, J.-M., Tran, H., Kuze,A., Keppel-Aleks, G., Toon, G., Wunch, D., Wennberg, P., Deutscher, N., Griffith, D., Macatangay, R., Messerschmidt, J., Notholt, J., and Warneke, T.: Toward accurate CO₂ and CH₄ observations from GOSAT, Geophys. Res. Lett., 38, L14812, https://doi.org/10.1029/2011GL047888, 2011.

Cogan et al., 2012: Cogan, A. J., Boesch, H., Parker, R. J., Feng, L., Palmer, P. I., Blavier, J.-F. L., Deutscher, N. M., Macatangay, R., Notholt, J., Roehl, C., Warneke, T., and Wunch, D.: Atmospheric carbon dioxide retrieved from the Greenhouse gases Observing SATellite (GOSAT): Comparison with ground-based TCCON observations and GEOS-Chem model calculations, J. Geophys. Res. Atmos., 117, D21301, https://doi.org/10.1029/2012JD018087, 2012.

Detmers, 2017a: R. Detmers, Algorithm Theoretical Basis Document (ATBD) – ANNEX B for products CO2_GOS_SRFP & CH4_GOS_SRFP, Copernicus Climate Change Service (C3S) project on satellitederived Essential Climate Variable (ECV) Greenhouse Gases (CO₂ and CH₄) data products (project C3S_312a_Lot6), Version 1 (21/08/2017), 2017.

Detmers, 2017b: R. Detmers, Algorithm Theoretical Basis Document (ATBD) – ANNEX C for product CH4_GOS_SRPR, Copernicus Climate Change Service (C3S) project on satellite-derived Essential Climate Variable (ECV) Greenhouse Gases (CO₂ and CH₄) data products (project C3S_312a_Lot6), Version 1 (21/08/2017), 2017.

O'Dell et al., 2012: O'Dell, C. W., Connor, B., Bösch, H., O'Brien, D., Frankenberg, C., Castano, R., Christi, M., Eldering, D., Fisher, B., Gunson, M., McDuffie, J., Miller, C. E., Natraj, V., Oyafuso, F., Polonsky, I., Smyth, M., Taylor, T., Toon, G. C., Wennberg, P. O., andWunch, D.: The ACOS CO₂ retrieval algorithm – Part 1: Description and validation against synthetic observations, Atmos. Meas. Tech., 5, 99–121, doi:10.5194/amt-5-99-2012, 2012.

Kiel et al., 2019: Kiel, M., O'Dell, C. W., Fisher, B., Eldering, A., Nassar, R., MacDonald, C. G., and Wennberg, P. O.: How bias correction goes wrong: measurement of XCO₂ affected by erroneous surface pressure estimates, Atmos. Meas. Tech., 12, 2241–2259, https://doi.org/10.5194/amt-12-2241-2019, 2019.

Krisna et al., 2021: Trismono Candra Krisna, Ilse Aben, Lianghai Wu, Otto Hasekamp, Jochen Landgraf: ESA Climate Change Initiative "Plus" (CCI+) Algorithm Theoretical Basis Document (ATBD) Version 1.3 – For the RemoTeC XCO2 and XCH4 GOSAT-2 SRON Full Physics Products

C3S2_312a_Lot2_DLR_2021SC1 - Product User Guide and Specification GHG ANNEX-D v7.2

(CO2_GO2_SRFP and CH4_GO2_SRFP) Version 2.0.0 for the Essential Climate Variable (ECV) Greenhouse Gases (GHG), https://www.iup.uni-bremen.de/carbon_ghg/docs/GHG-CCIplus/CRDP7/ATBDv3_GHG-CCI_CO2_CH4_GO2_SRFP_v2p0p0.pdf, 2021.

Reuter et al., 2010: M. Reuter, M. Buchwitz, O. Schneising, J. Heymann, H. Bovensmann, J. P. Burrows: A method for improved SCIAMACHY CO₂ retrieval in the presence of optically thin clouds. Atmospheric Measurement Techniques, 3, 209-232, 2010.

Reuter et al., 2011: M. Reuter, H. Bovensmann, M. Buchwitz, J. P. Burrows, B. J. Connor, N. M. Deutscher, D. W. T. Griffith, J. Heymann, G. Keppel-Aleks, J. Messerschmidt, J. Notholt, C. Petri, J. Robinson, O. Schneising, V. Sherlock, V. Velazco, T. Warneke, P. O. Wennberg, D. Wunch: Retrieval of atmospheric CO₂ with enhanced accuracy and precision from SCIAMACHY: Validation with FTS measurements and comparison with model results. Journal of Geophysical Research - Atmospheres, 116, D04301, doi: 10.1029/2010JD015047, 2011.

Reuter et al., 2013: M. Reuter, H. Bösch, H. Bovensmann, A. Bril, M. Buchwitz, A. Butz, J. P. Burrows, C. W. O'Dell, S. Guerlet, O. Hasekamp, J. Heymann, N. Kikuchi, S. Oshchepkov, R. Parker, S. Pfeifer, O. Schneising, T. Yokota, and Y. Yoshida: A joint effort to deliver satellite retrieved atmospheric CO₂ concentrations for surface flux inversions: the ensemble median algorithm EMMA. Atmospheric Chemistry and Physics, doi:10.5194/acp-13-1771-2013, 13, 1771-1780, 2013.

Reuter et al., 2016: M. Reuter, H. Bovensmann, M. Buchwitz, J. P. Burrows, J. Heymann, O. Schneising: Algorithm Theoretical Basis Document Version 5 (ATBDv5) - The Bremen Optimal Estimation DOAS (BESD) algorithm for the retrieval of XCO2 for the Essential Climate Variable (ECV) Greenhouse Gases (GHG), 2016.

Reuter et al., 2017a: M.Reuter, M.Buchwitz, O.Schneising, S.Noël, V.Rozanov, H.Bovensmann and J.P.Burrows: A Fast Atmospheric Trace Gas Retrieval for Hyperspectral Instruments Approximating Multiple Scattering - Part 1: Radiative Transfer and a Potential OCO-2 XCO₂ Retrieval Setup, Remote Sensing, 9(11), 1159; doi:10.3390/rs9111159, 2017.

Reuter et al., 2017b: M.Reuter, M.Buchwitz, O.Schneising, S.Noël, H.Bovensmann and J.P.Burrows: A Fast Atmospheric Trace Gas Retrieval for Hyperspectral Instruments Approximating Multiple Scattering - Part 2: Application to XCO₂ Retrievals from OCO-2, Remote Sensing, 9(11), 1102; doi:10.3390/rs9111102, 2017.

Reuter et al., 2020: M. Reuter, M. Buchwitz, O. Schneising, S. Noël, H. Bovensmann, J.P. Burrows, H. Boesch, A. Di Noia, J. Anand, R.J. Parker, P. Somkuti, L. Wu, O.P. Hasekamp, I. Aben, A. Kuze, H. Suto, K. Shiomi, Y. Yoshida, I. Morino, D. Crisp, C.W. O'Dell, J. Notholt, C. Petri, T. Warneke, V.A. Velazco, N.M. Deutscher, D.W.T. Griffith, R. Kivi, D.F. Pollard, F. Hase, R. Sussmann, Y.V. Té, K. Strong, S. Roche, M.K. Sha, M. De Mazière, D.G. Feist, L.T. Iraci, C.M. Roehl, C. Retscher, and D. Schepers: Ensemble-based satellite-derived carbon dioxide and methane column-averaged dry-air mole fraction data sets (2003-2018) for carbon and climate applications, Atmos. Meas. Tech., https://www.atmos-meas-tech.net/13/789/2020, 2020.

Reuter et al., 2021: M. Reuter, M. Hilker, S. Noël, M. Buchwitz, O. Schneising, H. Bovensmann, and J. P. Burrows: ESA Climate Change Initiative "Plus" (CCI+) Algorithm Theoretical Basis Document

Version 3 (ATBDv3) - Retrieval of XCO2 from the OCO-2 satellite using the Fast Atmospheric Trace Gas Retrieval (FOCAL) for the Essential Climate Variable (ECV) Greenhouse Gases (GHG), http://www.iup.uni-bremen.de/carbon_ghg/docs/GHG-CCIplus/CRDP7/ATBDv3_GHG-CCI_CO2_OC2_FOCA_v10.pdf, 2021.

Schneising et al. (2018): O. Schneising and the ESA CCI GHG project team: ESA Greenhouse Gases Climate Change Initiative (GHG_cci): Column-averaged CH₄ from SCIAMACHY generated with the WFMD algorithm (CH4_SCI_WFMD), version 4.0. Centre for Environmental Data Analysis, date of citation. https://catalogue.ceda.ac.uk/uuid/aa09603e91b44f3cb1573c9dd415e8a8, 2018.

Taylor et al., 2022: Taylor, T. E., O'Dell, C. W., Crisp, D., Kuze, A., Lindqvist, H., Wennberg, P. O., Chatterjee, A., Gunson, M., Eldering, A., Fisher, B., Kiel, M., Nelson, R. R., Merrelli, A., Osterman, G., Chevallier, F., Palmer, P. I., Feng, L., Deutscher, N. M., Dubey, M. K., Feist, D. G., García, O. E., Griffith, D. W. T., Hase, F., Iraci, L. T., Kivi, R., Liu, C., De Mazière, M., Morino, I., Notholt, J., Oh, Y.-S., Ohyama, H., Pollard, D. F., Rettinger, M., Schneider, M., Roehl, C. M., Sha, M. K., Shiomi, K., Strong, K., Sussmann, R., Té, Y., Velazco, V. A., Vrekoussis, M., Warneke, T., and Wunch, D.: An 11-year record of XCO2 estimates derived from GOSAT measurements using the NASA ACOS version 9 retrieval algorithm, Earth Syst. Sci. Data, 14, 325–360, https://doi.org/10.5194/essd-14-325-2022, 2022.

Yoshida et al., 2013: Yoshida, Y., Kikuchi, N., Morino, I., Uchino, O., Oshchepkov, S., Bril, A., Saeki, T., Schutgens, N., Toon, G. C., Wunch, D., Roehl, C. M., Wennberg, P. O., Griffith, D. W. T., Deutscher, N. M., Warneke, T., Notholt, J., Robinson, J., Sherlock, V., Connor, B., Rettinger, M., Sussmann, R., Ahonen, P., Heikkinen, P., Kyrö, E., Mendonca, J., Strong, K., Hase, F., Dohe, S., and Yokota, T.: Improvement of the retrieval algorithm for GOSAT SWIR XCO2 and XCH4 and their validation using TCCON data, Atmos. Meas. Tech., 6, 1533–1547, https://doi.org/10.5194/amt-6-1533-2013, 2013.

Yoshida and Oshio, 2020: Y. Yoshida and H. Oshio: GOSAT-2 TANSO-FTS-2 SWIR L2 Retrieval Algorithm Theoretical Basis Documen, National Institute for Environmental Studies, GOSAT-2 Project https://prdct.gosat-2.nies.go.jp/documents/pdf/ATBD_FTS-2_L2_SWL2_en_00.pdf, 2020.

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