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 (v4.3, 01/2003-06/2020)

C3S_312b_Lot2_DLR – Atmosphere

Issued by: Maximilian Reuter, University of Bremen,

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Contributors

INSTITUTE OF ENVIRONMENTAL PHYSICS (IUP), UNIVERSITY OF BREMEN, BREMEN, GERMANY

(IUP)

M. Reuter

M. Buchwitz

O. Schneising-Weigel

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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

Related documents

Reference ID	Document
D1	Main PUGS: **Buchwitz, M., et al.:** Product User Guide and Specification (PUGS) – Main document for Greenhouse Gas (GHG: CO2 & CH4) data set CDR 5 (01.2003-06.2020), project C3S_312b_Lot2_DLR – Atmosphere, v5.0, 2021. *(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 (v4.3, 01/2003-06/2020), project C3S_312b_Lot2_DLR – Atmosphere, v5.0, 2021.
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
CCI	Climate Change Initiative
CDR	Climate Data Record
CDS	(Copernicus) Climate Data Store
CMUG	Climate Modelling User Group (of ESA's CCI)
CRG	Climate Research Group
D/B	Data base
DOAS	Differential Optical Absorption Spectroscopy
EC	European Commission
ECMWF	European Centre for Medium Range Weather Forecasting
ECV	Essential Climate Variable
EMMA	Ensemble Median Algorithm
ENVISAT	Environmental Satellite (of ESA)
EO	Earth Observation
ESA	European Space Agency
EU	European Union
EUMETSAT	European Organisation for the Exploitation of Meteorological Satellites
FCDR	Fundamental Climate Data Record

FoM	Figure of Merit
FP	Full Physics retrieval method
FTIR	Fourier Transform InfraRed
FTS	Fourier Transform Spectrometer
GCOS	Global Climate Observing System
GEO	Group on Earth Observation
GEOSS	Global Earth Observation System of Systems
GHG	GreenHouse Gas
GOME	Global Ozone Monitoring Experiment
GMES	Global Monitoring for Environment and Security
GOSAT	Greenhouse Gases Observing Satellite
IASI	Infrared Atmospheric Sounding Interferometer
IMAP-DOAS (or IMAP)	Iterative Maximum A posteriori DOAS
IPCC	International Panel in Climate Change
IUP	Institute of Environmental Physics (IUP) of the University of Bremen, Germany
JAXA	Japan Aerospace Exploration Agency
JCGM	Joint Committee for Guides in Metrology
L1	Level 1
L2	Level 2
L3	Level 3
L4	Level 4
LMD	Laboratoire de Météorologie Dynamique
MACC	Monitoring Atmospheric Composition and Climate, EU GMES project
NA	Not applicable
NASA	National Aeronautics and Space Administration
NetCDF	Network Common Data Format
NDACC	Network for the Detection of Atmospheric Composition Change

NIES	National Institute for Environmental Studies
NIR	Near Infra Red
NLIS	LMD/CNRS *neuronal* network mid/upper tropospheric CO2 and CH4 retrieval algorithm
NOAA	National Oceanic and Atmospheric Administration
Obs4MIPs	Observations for Climate Model Intercomparisons
OCO	Orbiting Carbon Observatory
OE	Optimal Estimation
PBL	Planetary Boundary Layer
ppb	Parts per billion
ppm	Parts per million
PR	(light path) PRoxy retrieval method
PVIR	Product Validation and Intercomparison Report
QA	Quality Assurance
QC	Quality Control
REQ	Requirement
RMS	Root-Mean-Square
RTM	Radiative transfer model
SCIAMACHY	SCanning Imaging Absorption spectroMeter for Atmospheric ChartographY
SCIATRAN	SCIAMACHY radiative transfer model
SRON	SRON Netherlands Institute for Space Research
SWIR	Short Wava Infra Red
TANSO	Thermal And Near infrared Sensor for carbon Observation
TANSO-FTS	Fourier Transform Spectrometer on GOSAT
TBC	To be confirmed
TBD	To be defined / to be determined
TCCON	Total Carbon Column Observing Network
TIR	Thermal Infra Red

TR	Target Requirements
TRD	Target Requirements Document
WFM-DOAS (or WFMD)	Weighting Function Modified DOAS
UoL	University of Leicester, United Kingdom
URD	User Requirements Document
WMO	World Meteorological Organization
Y2Y	Year-to-year (bias variability)

General definitions

Table 1 lists some general definitions relevant for this document.

Table 1: General definitions.

Item	Definition
XCO2	Column-averaged dry-air mixing ratios (mole fractions) of CO_2
XCH4	Column-averaged dry-air mixing ratios (mole fractions) of CH_4
L1	Level 1 satellite data product: geolocated radiance (spectra)
L2	Level 2 satellite-derived data product: Here: XCO2 and XCH4 information for each ground-pixel
L3	Level 3 satellite-derived data product: Here: Gridded XCO2 and XCH4information, e.g., 5°x5°, monthly
L4	Level 4 satellite-derived data product: Here: Surface fluxes (emission and/or uptake) of CO_2 and CH_4

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 C3S_312b_Lot2.

Within this project satellite-derived atmospheric carbon dioxide (CO_2) and methane (CH_4) 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_2 and CH_4, denoted XCO_2 (in parts per million, ppm) and XCH_4 (in parts per billion, ppb), respectively.
- Mid/upper tropospheric mixing ratios of CO_2 (in ppm) and CH_4 (in ppb).

This document describes the C3S products XCO2_EMMA, XCH4_EMMA, XCO2_OBS4MIPS, and XCH4_OBS4MIPS.

These products are merged multi-sensor XCO_2 and XCH_4 Level 2 and Level 3 products generated using algorithms developed at University of Bremen, Germany (see *D2*).

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_2 or XCH_4 satellite retrieval, i.e., the EMMA database includes all information needed for inverse modeling (geo-location, time, XCO_2 or XCH_4, 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_2 and XCH_4 L2 data sets provided by the Copernicus C3S_312b_Lot2 sub-project.

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 subject to this ANNEX describing the EMMA v4.3 CO_2 and EMMA v4.3 CH_4 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*).

1. Product description

1.1 EMMA products

Additionally to the common variables described in the main PUGS document (*D1*) the EMMA L2 data base includes the variables listed in **Table 2** and described in the following. **Table 3** lists all individual sensor / individual algorithm Level 2 products, which have been used as input for the generation of the EMMA XCO_2 and XCH_4 products.

Table 2: EMMA v4.3 CO_2 and EMMA v4.3 CH_4 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	For XCO2: ppm, i.e., 10^{-6} For XCH4: 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_se	Float	n	For XCO2: ppm, i.e., 10^{-6} For XCH4: ppb, i.e., 10^{-9}	Standard error of the median uncertainty (see *D2*)
median_uncertainty_ex	Float	n	For XCO2: ppm, i.e., 10^{-6} For XCH4: ppb, i.e., 10^{-9}	Inter-algorithm spread as expected from measurement noise (see *D2*)
<xco2|xch4>_accuracy	Float	n	For XCO2: ppm, i.e., 10^{-6} For XCH4: ppb, i.e., 10^{-9}	Potential spatio/temporal XCO2 or XCH4 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 v4.3 CO_2 and CH_4. See listing in **Table 3**.

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|xch4>_accuracy

Potential spatio/temporal XCO2 or 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.

Table 3: Unique L2 algorithm IDs used in EMMA v4.3 CO_2 and CH_4.

ID	Quantity	Instrument	Name	Version	Institution
2	XCO2	SCIAMACHY	BESD	v02.01.02	IUP
2000	XCO2	TANSO-FTS	FOCAL	V1.0	IUP
3	XCO2	TANSO-FTS	ACOS	v9r	NASA
4	XCO2	TANSO-FTS	RemoTeC	v2.3.8	SRON
6	XCO2	TANSO-FTS	UoL-FP	v7.3	UoL
-6	XCO2	TANSO-FTS	PPDF-S	v02.xx	NIES
5	XCO2	TANSO-FTS	NIES	v02.9xbc (bias corrected)	NIES
1000	XCO2	OCO-2	FOCAL	v09	IUP
10	XCO2	OCO-2	NASA	V10.2	NASA
30	XCH4	TANSO-FTS	RemoTeC-PR	v2.3.9	SRON
31	XCH4	TANSO-FTS	RemoTeC-FP	v2.3.8	SRON
40	XCH4	TANSO-FTS	UoL-PR	V9.0	UoL
41	XCH4	TANSO-FTS	UoL-FP	v7.3	UoL
50	XCH4	TANSO-FTS	PPDF-S	v02.xx	NIES
60	XCH4	TANSO-FTS	NIES	v02.9xbc (bias corrected)	NIES
70	XCH4	SCIAMACHY	WFMD	v4.0	IUP

1.2 OBS4MIPS products

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

The XCO2_OBS4MIPS and XCH4_OBS4MIPS data products are in Obs4MIPs NCDF format, which is described on the Obs4MIPs website: https://www.earthsystemcog.org/projects/obs4mips/.

The XCO2_OBS4MIPS and XCH4_OBS4MIPS products are generated by spatial (5°x5°) and temporal (monthly) gridding of the corresponding EMMA L2 products.

The OBS4MIPS L3 products include the variables listed in **Table 4** and described in the following.

Table 4: XCO2_OBS4MIPS and XCH4_OBS4MIPS variables. x, y, z, t, represent the number of grid points in longitude, latitude, pressure, and temporal direction.

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|xch4>	Float	x,y,t	1	Satellite retrieved column-average dry-air mole fraction of CO2 or CH4
<xco2|xch4>_nobs	Integer	x,y,t	1	Number of individual L2 observations
<xco2|xch4>_stdder	Float	x,y,t	1	Standard error
<xco2|xch4>_stddev	Float	x,y,t	1	Standard deviation
column averaging kernel	Float	x,y,z,t	1	Column-averaging kernel
vmr_profile_<co2|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.

<xco2|xch4>

Main parameter: satellite retrieved column-average dry-air mole fraction of CO_2 or CH_4.

<xco2|xch4>_nobs

Number of individual L2 observations per grid box.

<xco2|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.

<xco2|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 XCO_2 or XCH_4 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|ch4>_apriori

A priori dry-air mole fraction profile of atmospheric CO_2 or CH_4. 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.

2. Target requirements

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

3. Data usage information

3.1 EMMA products

The EMMA database consists of individual level 2 soundings which can be used in the same manner as any other XCO_2 or XCH_4 satellite retrieval, i.e., the EMMA database includes all information needed for inverse modelling (geo-location, time, XCO_2 or XCH_4, averaging kernels, etc.). The main PUGS document (*D1*) provides guidance on how to use the information.

Figure 1 shows for an example month (April 2015) the EMMA XCO_2 and XCH_4 and the corresponding algorithm selected by the median (see *D2*). **Figure 2** shows the average inter-algorithm spread (01/2003 – 06/2020) and the expected average inter-algorithm spread due to measurement noise for XCO_2 and XCH_4.

Figure 1: EMMA L2 XCO_2 and XCH_4 (**left**) and corresponding selected algorithm (**right**) for EMMA v4.3 CO_2 (**top**) and EMMA v4.3 CH_4 (**bottom**) at the example of April 2015.

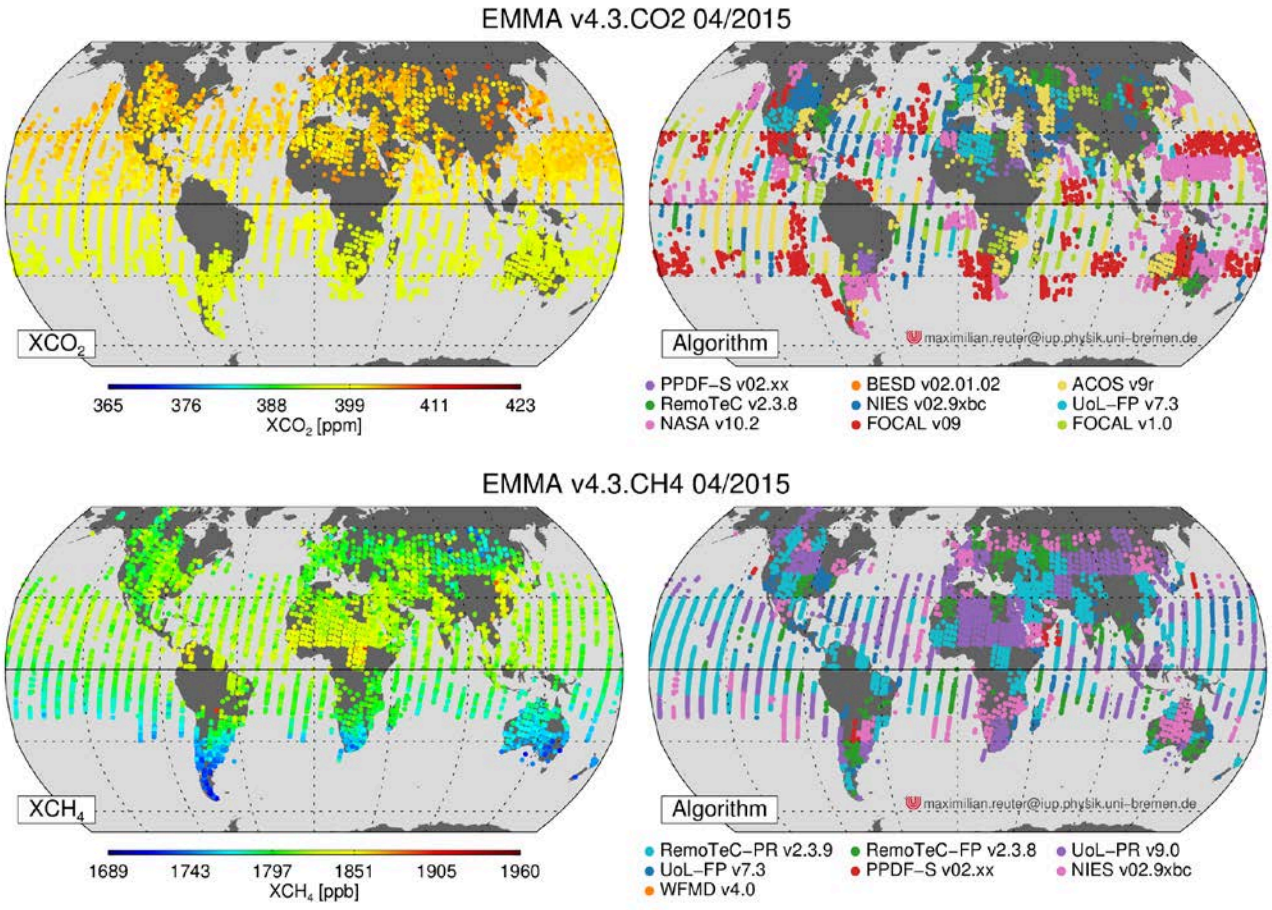
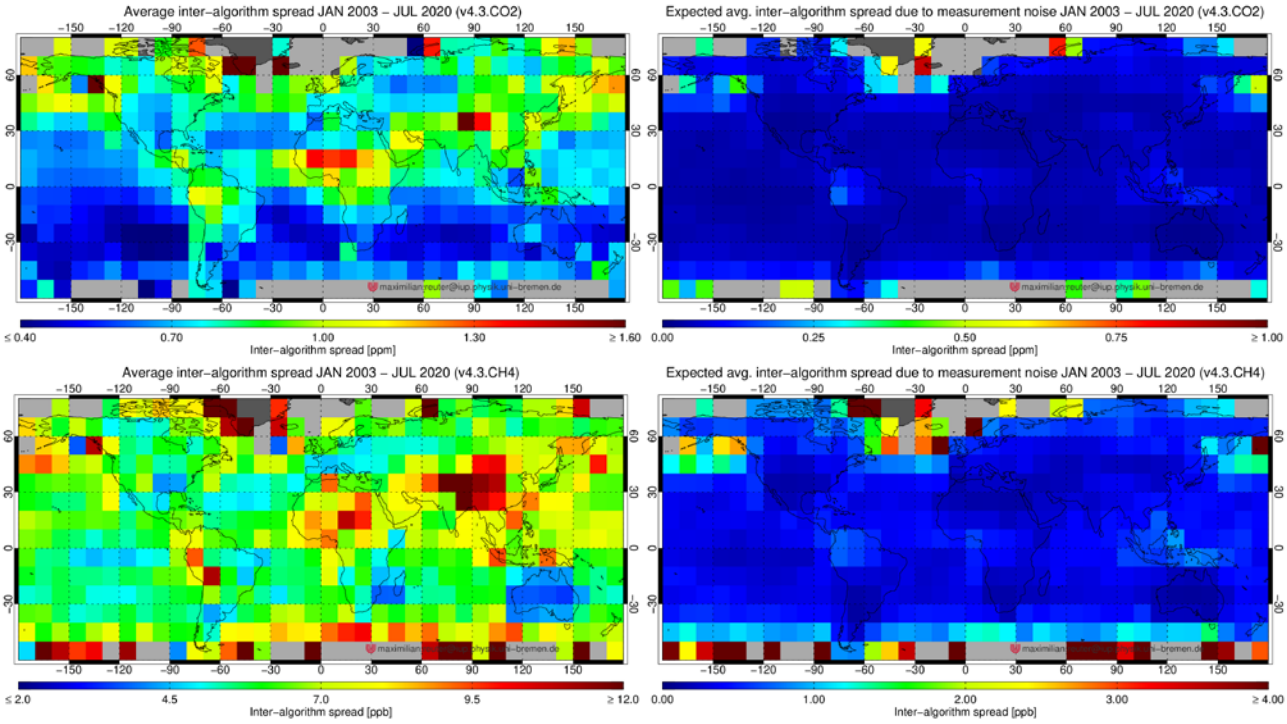


Figure 2: Average inter-algorithm spread (01/2003 – 06/2020) (**left**) and expected average inter-algorithm spread due to measurement noise (**right**) for EMMA v4.3 CO_2 (**top**) and EMMA v4.3 CH_4 (**bottom**).

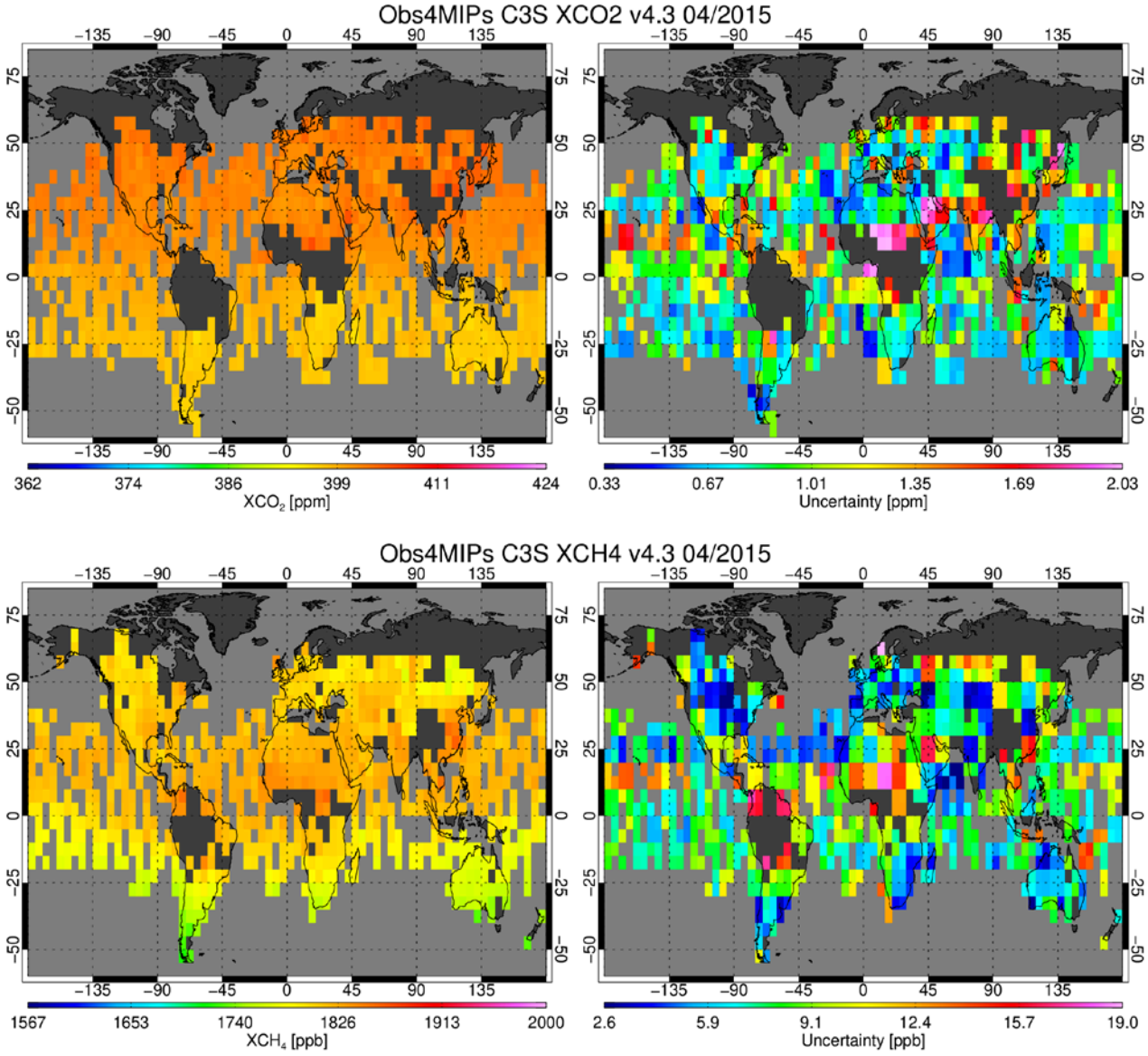


3.2 OBS4MIPS products

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_2 or XCH_4 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 3 shows for an example month (April 2015) the OBS4MIPS XCO_2 and XCH_4 and the corresponding uncertainty computed from the retrieval noise and EMMA's inter-algorithm spread (see *D2*).

Figure 3: Top: XCO2_OBS4MIPS XCO_2 for April 2015 (**left**) and its uncertainty computed from the retrieval noise and EMMA's inter-algorithm spread (**right**). **Bottom**: Same for XCH4_OBS4MIPS.



Copernicus Climate Change Service

ECMWF - Shinfield Park, Reading RG2 9AX, UK

Contact: info@copernicus-climate.eu

climate.copernicus.eu copernicus.eu ecmwf.int