



Product User Guide and Specification (PUGS) – ANNEX B for products CO2_GO2_SRF, CH4_GO2_SRF (v2.0.0, 2019-2021)

C3S2_312a_Lot2_DLR – Atmosphere

Issued by: Andrew Barr and Tobias Borsdorff, SRON, The Netherlands

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Contributors

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

M. Buchwitz

**SRON NETHERLANDS INSTITUTE FOR SPACE RESEARCH,
LEIDEN, THE NETHERLANDS
(SRON)**

T. Borsdorff

A. G. Barr

O. P. Hasekamp



History of modifications

Version	Date	Description of modification	Chapters / Sections
1.3	20-October-2017	New document for data set CDR1 (2009-2016)	All
2.0	4-October-2018	Update for CDR2 (2009-2017)	All
3.0	12-August-2019	Update for CDR3 (2009-2018)	All
3.1	03-November-2019	Update after review by Assimila: Correction of typos.	All
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4.0	18-August-2020	Update for CDR4 (2009-2019)	All
5.0	18-February-2021	Update for CDR5 (2009-mid2020)	All
6.0	4-August-2022	Update for CDR6: GOSAT-2 retrievals (2019 - 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



List of datasets covered by this document

Deliverable ID	Product title	Product type (CDR, ICDR)	Version number	Delivery date
WP2-FDDP-GHG-v1	CO2_GO2_SRF	CDR 6	2.0.0	31-Aug-2022
WP2-FDDP-GHG-v1	CH4_GO2_SRF	CDR 6	2.0.0	31-Aug-2022

Related documents

Reference ID	Document
D1	<p>Main PUGS: Buchwitz, M., et al., Product User Guide and Specification (PUGS) – Main document for Greenhouse Gas (GHG: CO₂ & CH₄) 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>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 (CO₂ and CH₄) data products (project C3S_312b_Lot2), Version 2.11, 9-April-2020, pp. 80, 2020.</p>
D3	<p>Barr, A. G., et al., Algorithm Theoretical Basis Document (ATBD) – ANNEX B for product CH₄ GO₂ SRF and CO₂ SRF (v2.0.0, 2019-2021), Technical Report C3S project C3S2 312a Lot2 DLR – Atmosphere, version 6.2, 2023.</p>



Acronyms

Acronym	Definition
ATBD	Algorithm Theoretical Basis Document
CAR	Climate Assessment Report
C3S	Copernicus Climate Change Service
CCI	Climate Change Initiative
CDR	Climate Data Record
CDS	(Copernicus) Climate Data Store
CRG	Climate Research Group
D/B	Data base
EC	European Commission
ECMWF	European Centre for Medium Range Weather Forecasting
ECV	Essential Climate Variable
EO	Earth Observation
ESA	European Space Agency
EU	European Union
EUMETSAT	European Organisation for the Exploitation of Meteorological Satellites
FP	Full Physics retrieval method
FTIR	Fourier Transform InfraRed
FTS	Fourier Transform Spectrometer
GCOS	Global Climate Observing System
GEOSS	Global Earth Observation System of Systems
GHG	GreenHouse Gas
GOSAT	Greenhouse Gases Observing Satellite
GOSAT-2	Greenhouse Gases Observing Satellite 2
IPCC	International Panel in Climate Change
IUP	Institute of Environmental Physics (IUP) of the University of Bremen, Germany
JAXA	Japan Aerospace Exploration Agency
KIT	Karlsruhe Institute of Technology
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
NetCDF	Network Common Data Format
NIES	National Institute for Environmental Studies
NIR	Near Infra Red



NOAA	National Oceanic and Atmospheric Administration
Obs4MIPs	Observations for Climate Model Intercomparisons
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
RemoTeC	Retrieval algorithm developed by SRON
REQ	Requirement
RMS	Root-Mean-Square
RTM	Radiative transfer model
SNR	Signal-to-Noise Ratio
SRON	SRON Netherlands Institute for Space Research
SWIR	Short Wave Infra Red
SZA	Solar Zenith Angle
TANSO	Thermal And Near infrared Sensor for carbon Observation
TANSO-FTS	Fourier Transform Spectrometer on GOSAT
TANSO-FTS-2	Fourier Transform Spectrometer on GOSAT-2
TBC	To be confirmed
TBD	To be defined / to be determined
TCCON	Total Carbon Column Observing Network
TIR	Thermal Infra Red
TR	Target Requirements
TRD	Target Requirements Document
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, <http://climate.copernicus.eu/>) 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 have been 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 GHG satellite-derived 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 C3S2 products CO₂_GO2_SRFP and CH₄_GO2_SRFP v2.0.0.

These products are XCO₂ and XCH₄ Level 2 products as retrieved from GOSAT-2 using algorithms developed at SRON, The Netherlands.



Executive summary

Because of their important role for climate, they are classified as Essential Climate Variables (ECVs). The ECV GHG as formulated by GCOS (Global Climate Observing System) is defined as follows: “Retrievals of greenhouse gases, such as CO₂ and CH₄, of sufficient quality to estimate regional sources and sinks” (GCOS-154). This definition contains already the main application of these atmospheric data products; namely to use them (in combination with appropriate modelling) to obtain (improved) information on their (primarily surface) sources and sinks.

Both gases (CO₂ and CH₄) have a long lifetime in the atmosphere. As a consequence of this fact and related human emissions, the atmospheric concentrations of these gases are relatively high compared to other atmospheric trace gases. As a result of this, even a moderate to strong (surface) source or sink typically only results in a relatively small local or regional change (enhancement or depletion relative to the surrounding region) in their vertical columns or their mid/upper tropospheric concentration. The observational requirements are therefore very demanding in particular with respect to random and systematic errors and stability.

This document is Annex B of the Product User Guide (PUG), which is a deliverable of the C3S2 project. This document describes the XCO₂ and XCH₄ Full Physics data products generated by the RemoTeC algorithm (CO₂_GO₂_SRFP and CH₄_GO₂_SRFP). The description includes quality flags, metadata, data format, product grid, defined limitations, bias correction, and the product (column) averaging kernels, as well as a description of how to use them appropriately.

The greenhouse gas (GHG) activities of this C3S project and its C3S pre-cursor projects are essentially the operational continuation of the research and development (R&D) pre-cursor projects GHG-CCI and GHG-CCI+ of ESA’s Climate Change Initiative (CCI). R&D for the GOSAT-2 products is currently an ongoing activity of the ESA GHG-CCI+ project*.

The description includes quality flags and metadata, data format, product grid, known limitations, bias correction, and the product (column) averaging kernels and a description of how to use them. The two data products (XCO₂ and XCH₄) are produced by the same retrieval, and separated into different products in the post-processing therefore in the following sections, we treat both products as one, and give the necessary details for each where necessary.

Section 1.1 describes the product, covering the relevant information for the algorithm and input data, as well as describing the bias correction process. Section 1.2 presents the target requirements for these products, and section 1.3 outlines how to use the data. Finally, section 2 provides information on where to find, and how to access, the data.

*<http://climate.esa.int/en/projects/ghgs/> - 16 Jan 2023



1. Full Physics Products

1.1 Data product description

The Japanese Greenhouse gases Observing SATellite-2 (GOSAT-2) was launched on 29th October 2018 and started operational observations from February 2019. GOSAT-2 provides dedicated global measurements of total column CO₂ and CH₄ from its SWIR bands. It is equipped with two instruments, the Thermal And Near Infrared Sensor for carbon Observations - Fourier Transform Spectrometer-2 (TANSO-FTS2) with spectral channels presented in Table 1. A more extensive description of the instrument can be found in the ATBD Annex-B (D3 in the related documents section).

Table 1: GOSAT-2-FTS bands.

Channel	Wavelength range [nm]	Resolution [cm ⁻¹]
1	758-775	0.2
2	1460-1720	0.2
3	1920-2330*	0.2
4	5560-8400	0.2
5	8400-14300	0.2

*GOSAT-1 only had a spectral range up to 2080nm.

The CH₄_GO2_SRFP and CO₂_GO2_SRFP products are retrieved from GOSAT-2 TANSO-FTS-2 NIR and SWIR spectra using the RemoTeC algorithm that is being jointly developed at SRON and KIT. The algorithm retrieves simultaneously XCH₄ and XCO₂. For the retrieval, we analyze four spectral regions: the 0.77 μm oxygen band, two CO₂ bands at 1.61 and 2.06 μm, as well as a CH₄ band at 1.64 μm. Within the retrieval procedure the sub-columns of CO₂ and CH₄ in different altitude layers are being retrieved. To obtain the column averaged dry air mixing ratios XCO₂ and XCH₄ the sub-columns are summed up to get the total column which is divided by the dry-air columns obtained from ECMWF model data in combination with a surface elevation data base. The retrieved XCH₄ and XCO₂ have been extensively validated with ground based Total Carbon Column Observing Network (TCCON) measurements. To further improve accuracy a bias correction has been developed based on TCCON comparisons. We use the GGG2020 TCCON dataset.

More details on the technical aspects of the retrievals and auxiliary data can be found in the ATBD Annex-B (D3).



1.1.1 Bias Correction

From comparison with TCCON (Wunch et al. 2015) it was found that the error in XCH4 correlates with the retrieved albedo α at 1.6 μm in band 2. Based on this correlation the following bias correction has been developed for XCO2:

$$XCO2_{corr} = XCO2 * (a + b * \alpha) \quad (1)$$

with $a=0.99046$ and $b=0.05202$ for land (normal) data and $a = 1.00316$, $b = -0.04484$ for ocean (sunlint) data.

The bias correction parameters are obtained from fits to the GOSAT-2-TCCON differences and the subsequent correlation with TCCON is illustrated in Figure 1.

Similarly, for XCH4 it was found that the error in XCH4 correlates with the albedo α at 1.6 μm in band 2. Based on this correlation the following bias correction has been developed for XCH4:

$$XCH4_{corr} = XCH4 * (a + b * \alpha) \quad (2)$$

with $a = 0.99334$, $b = 0.03448$ for land (normal) data and $a = 0.99994$ and $b = -0.03865$ for ocean (sunlint) data

The bias correction parameters are obtained from fits to the GOSAT-2-TCCON differences and the subsequent correlation with TCCON is illustrated in Figure 2.

Figures 3 and 4 show global maps of XCO2 and XCH4, respectively, for land (normal) and ocean (sunlint) soundings separately. These have been sampled onto a 1x1 degree grid and cover the entire time range of available GOSAT-2 data.



Figure 1: Co-located GOSAT-2-TCCON XCO₂ measurements for land (normal) measurements

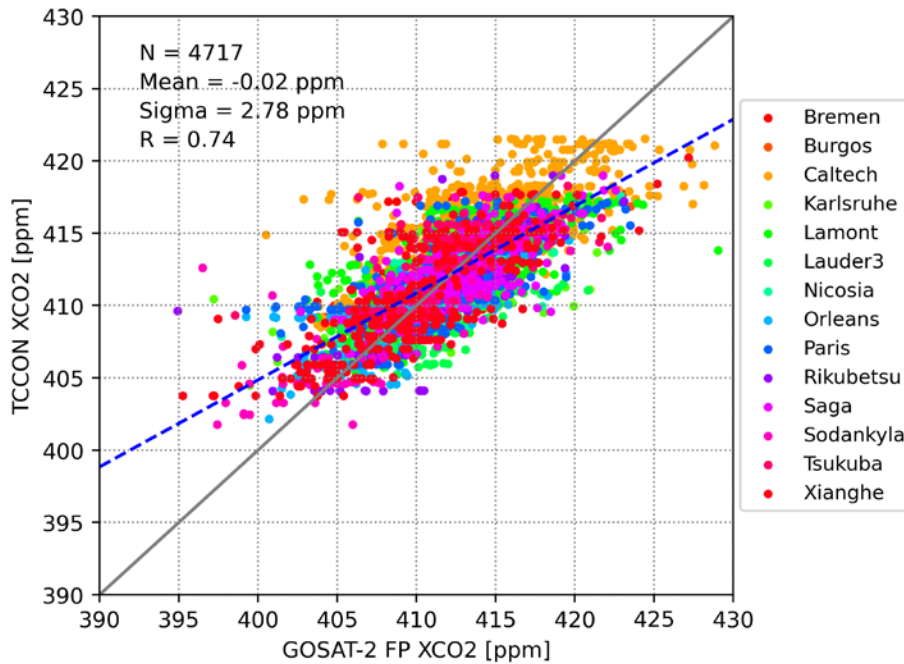


Figure 2: Co-located GOSAT-2-TCCON XCH₄ measurements for land (normal) measurements

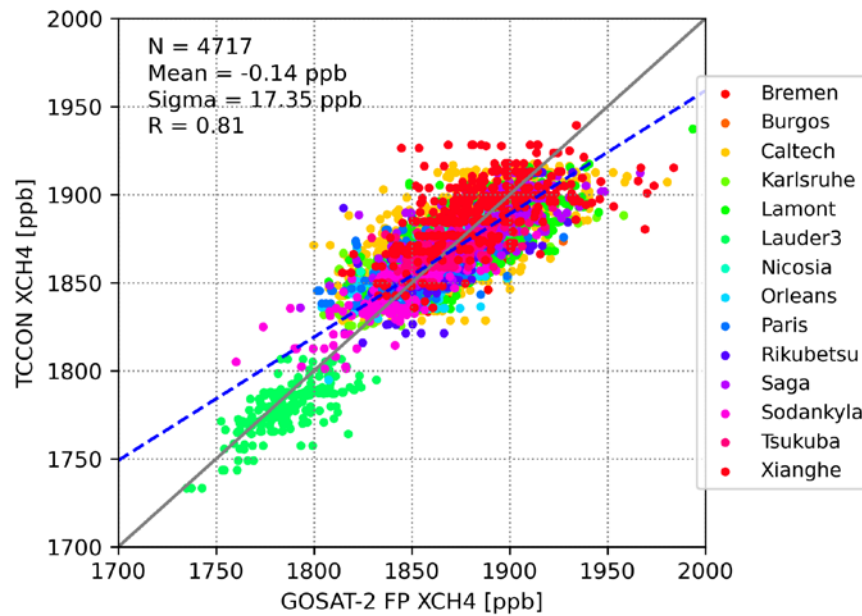




Figure 3: Global XCO₂ for the 2019-2021 period for the CO₂_GO₂_SRFP product on a 1 by 1 degree resolution for both land (normal) (top) and ocean (sun glint) (bottom) soundings.

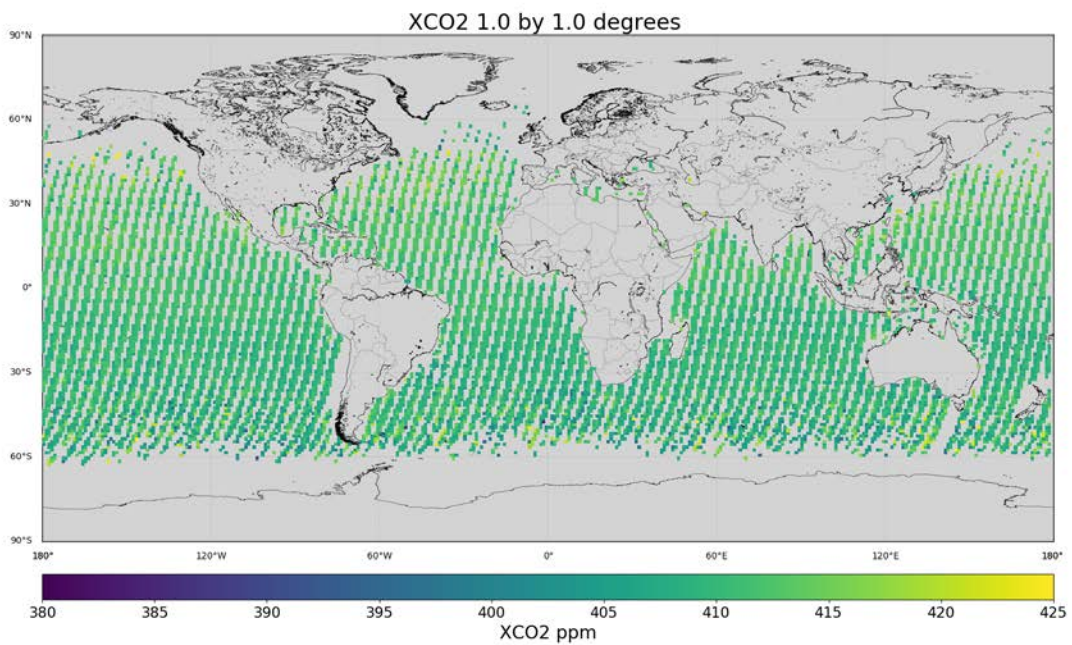
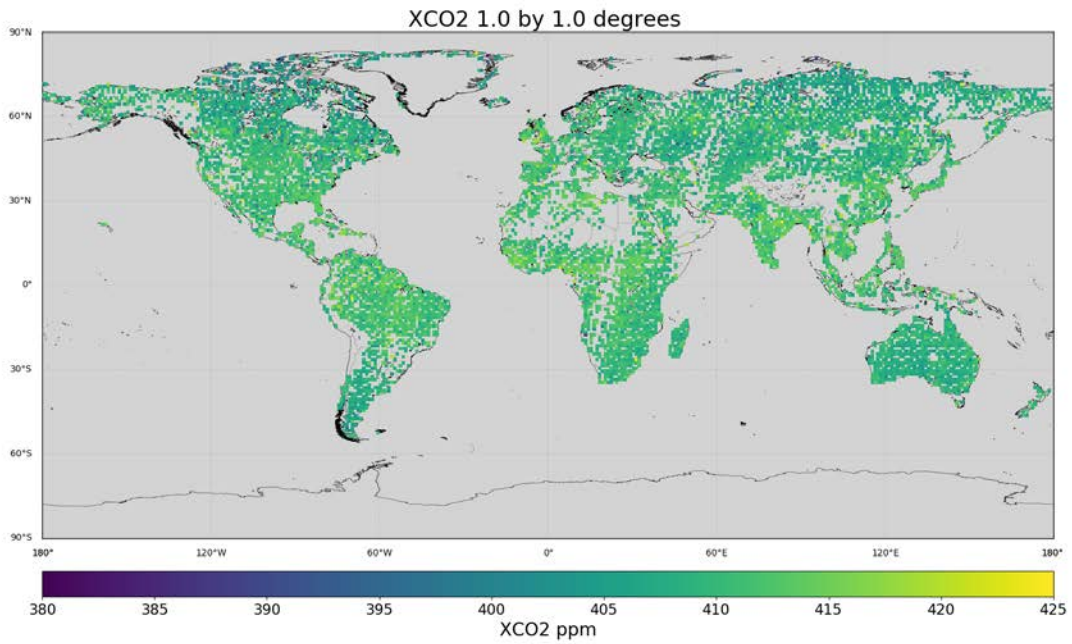
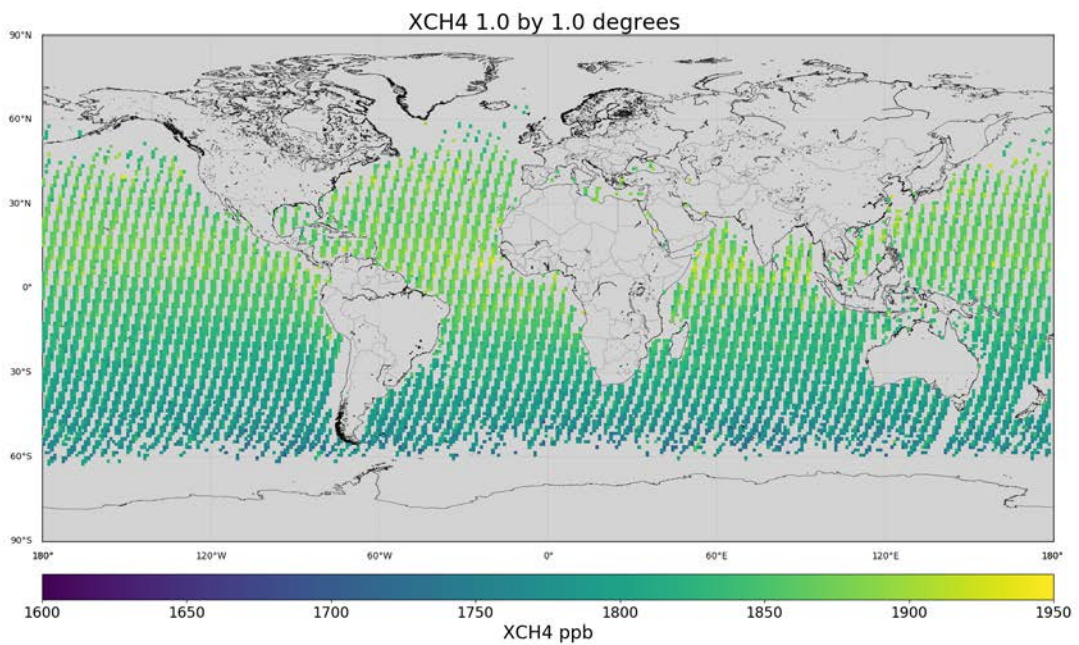
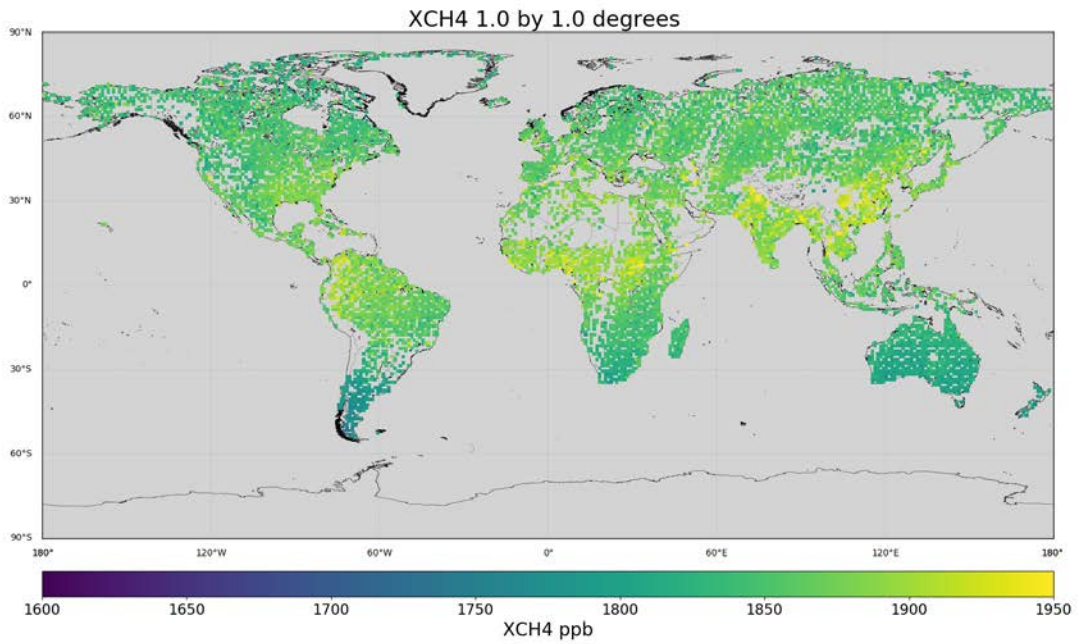




Figure 4: Global XCH4 for the 2019-2021 period for the CH4_GO2_SRFP product on a 1 by 1 degree resolution for both land (normal) (top) and ocean (sunglint) (bottom) soundings.





1.2 Target requirements

The target requirements for the products in this document are taken from the Target Requirements Document (D2) for greenhouse gas retrievals and presented in Table 2. CO₂ and CH₄ are important climate-relevant atmospheric gases, so-called greenhouse gases (GHG). Because of their important role for climate, they are classified as Essential Climate Variables (ECVs). The ECV GHG as formulated by GCOS (Global Climate Observing System) is defined as follows: “Retrievals of greenhouse gases, such as CO₂ and CH₄, of sufficient quality to estimate regional sources and sinks” (GCOS-154). This definition contains already the main application of these atmospheric data products; namely to use them (in combination with appropriate modelling) to obtain (improved) information on their (primarily surface) sources and sinks.

Both gases (CO₂ and CH₄) have lifetimes in the atmosphere of hundreds of years and 10-15 years, respectively. As a consequence of this fact and related human emissions, the atmospheric concentrations of these gases are relatively high compared to other atmospheric trace gases. As a result of this, even a moderate to strong (surface) source or sink typically only results in a relatively small local or regional change (enhancement or depletion relative to the surrounding region) in their vertical columns or their mid/upper tropospheric concentration. The observational requirements are therefore very demanding in particular with respect to random and systematic errors and stability.

Table 2: Goal (G), breakthrough (B) and threshold (T) target requirements for XCH₄ and XCO₂.

Random and systematic error requirements for XCO ₂ and XCH ₄					
Parameter	Req. type	Random error (“Precision”)		Systematic error	Stability
		Single obs.	1000 ² km ² monthly		
XCO ₂	G	< 1 ppm	< 0.3 ppm	< 0.2 ppm (absolute)	As systematic error but per year
	B	< 3 ppm	< 1.0 ppm	< 0.3 ppm (relative)	“-”
	T	< 8 ppm	< 1.3 ppm	< 0.5 ppm (relative)	“-”
XCH ₄	G	< 9 ppb	< 3 ppb	< 1 ppb (absolute)	< 1 ppb/year (absolute)
	B	< 17 ppb	< 5 ppb	< 5 ppb (relative)	< 2 ppb/year (relative)
	T	< 34 ppb	< 11 ppb	< 10 ppb (relative)	< 3 ppb/year (relative)



1.3 Data usage information

1.3.1 Product Content and Format

The CH₄_GO₂_SRFP and CO₂_GO₂_SRFP v2.0.0 data products are stored per day in a single NetCDF (version 4) file. Retrieval results are provided for the individual GOSAT-2 spatial footprints, i.e., no averaging has been applied. The product file contains a set of common variables, i.e., the retrieved column averaged dry air mixing ratios XCO₂ and XCH₄ with bias correction, averaging kernels and quality flags, as well as secondary variables specific for the RemoTeC algorithm. Common and retrieval-specific variables for the XCO₂ product are given in Tables 3 and 4, respectively. Common and retrieval-specific variables for the XCH₄ product are given in Tables 5 and 6, respectively.

Table 3: Common variables for the CO₂_GO₂_SRFP product

Name	Type	Dim.	Units	Description
solar_zenith_angle	float	n	degrees	Angle between line of sight to the sun and local vertical
sensor_zenith_angle	float	n	degrees	Angle between the line of sight to the sensor and the local vertical
time	float	n	seconds	Seconds since 1970-01-01 00:00:00
longitude	float	n	degrees_ east	Center longitude
latitude	float	n	degrees_ north	Center latitude
pressure_levels	float	n, 13	hPa	Pressure levels
pressure_weight	float	n, 12		Layer dependent weights needed to apply the averaging kernels
xco2	float	n	1e-6	Retrieved column dry-air mole fraction of atmospheric carbon dioxide (XCO ₂) in ppm
xco2_uncertainty	float	n	1e-6	1-sigma uncertainty of the retrieved column-average dry-air mole fraction of atmospheric carbon dioxide
xco2_averaging_kernel	float	n, 12		Normalized column averaging kernel
co2_profile_apriori	float	n, 12	1e-6	A priori dry-air mole fraction profile of atmospheric carbon dioxide
xco2_quality_flag	int	n		Quality flag for XCO ₂ retrieval, 0 = good, 1 = bad



Table 4: Product specific (additional) variables for the CO2_GO2_SRFP product

Name	Type	Dim.	Units	Description
flag_landtype	int	n		0 = land, 1 = ocean
flag_sunlint	int	n		0 = no sunlint, 1 = sunlint
gain	char	n		Number of gain coefficient calculated from solar calibration mode data. [1P 1S 2P 2S 3P 3S]
exposure_id	int	n		Exposure identification number of the sounding
l1b_name	char	n		Name of the Level 1B file of the sounding
signal_to_noise_window	float	n, 4, 2		Signal to noise ratio per retrieval window and for both polarization directions
dry_airmass_layer	float	n, 12	m-2	Dry airmass per layer
altitude	float	n	m	Vertical distance above the surface
air_temperature	float	n, 13	K	The bulk temperature of the air at each level
surface_elevation_stdev	float	n	m	Standard deviation of the surface elevation within the sounding
x_wind	float	n, 13	m s-1	Eastward wind velocity
y_wind	float	n, 13	m s-1	Northward wind velocity
chi2	float	n		Chi-squared value of the sounding
optical_thickness_of_atmosphere_layer_due_to_ambient_aerosol	float	n, 4		Scattering optical thickness per retrieval window
raw_xco2	float	n	1e-6	Retrieved column dry-air mole fraction of atmospheric carbon dioxide (XCO2) in ppm before bias correction
raw_xco2_err	float	n	1e-6	1-sigma statistical uncertainty of the retrieved column-average dry-air mole fraction of atmospheric carbon dioxide
h2o_column	float	n	m-2	Retrieved total water column
surface_albedo_758	float	n		The retrieved albedo at 758 nm
surface_albedo_1593	float	n		The retrieved albedo at 1593 nm
surface_albedo_1629	float	n		The retrieved albedo at 1629 nm
surface_albedo_2042	float	n		The retrieved albedo at 2042 nm
intensity_offset_o2a	float	n	W cm-2	The retrieved intensity offset in the O2A band
aerosol_size	float	n		Retrieved size parameter of the aerosol distribution
aerosol_central_height	float	n	m	Peak height of the aerosol Gaussian height distribution
aerosol_total_column	float	n	m-2	Retrieved total aerosol column



Table 5: Common variables for the CH4_GO2_SRFP product

Name	Type	Dim.	Units	Description
solar_zenith_angle	float	n	degrees	Angle between line of sight to the sun and local vertical
sensor_zenith_angle	float	n	degrees	Angle between the line of sight to the sensor and the local vertical
time	float	n	seconds	Seconds since 1970-01-01 00:00:00
longitude	float	n	degrees_east	Center longitude
latitude	float	n	degrees_north	Center latitude
pressure_levels	float	n, 13	hPa	Pressure levels
pressure_weight	float	n, 12		Layer dependent weights needed to apply the averaging kernels
xch4	float	n	1e-9	Retrieved column dry-air mole fraction of atmospheric methane (XCH4) in ppb
xch4_uncertainty	float	n	1e-9	1-sigma uncertainty of the retrieved column-average dry-air mole fraction of atmospheric methane
xch4_averaging_kernel	float	n, 12		Normalized column averaging kernel
ch4_profile_apriori	float	n, 12	1e-9	A priori dry-air mole fraction profile of atmospheric methane
xch4_quality_flag	int	n		Quality flag for XCH4 retrieval, 0 = good, 1 = bad



Table 6: Product specific (additional) variables for the CH4_GO2_SRFP product

Name	Type	Dim.	Units	Description
flag_landtype	int	n		0 = land, 1 = ocean
flag_sunlint	int	n		0 = no sunlint, 1 = sunlint
gain	char	n		Number of gain coefficient calculated from solar calibration mode data. [1P 1S 2P 2S 3P 3S]
exposure_id	int	n		Exposure identification number of the sounding
l1b_name	char	n		Name of the Level 1B file of the sounding
signal_to_noise_window	float	n, 4, 2		Signal to noise ratio per retrieval window and for both polarization directions
dry_airmass_layer	float	n, 12	m-2	Dry airmass per layer
altitude	float	n	m	Vertical altitude above the surface
air_temperature	float	n, 13	K	The bulk temperature of the air at each level
surface_altitude_stdev	float	n	m	Standard deviation of the surface elevation within the sounding
x_wind	float	n, 13	m s-1	Eastward wind velocity
y_wind	float	n, 13	m s-1	Northward wind velocity
chi2	float	n		Chi-squared value of the sounding
optical_thickness_of_atmosphere_layer_due_to_ambient_aerosol	float	n, 4		Scattering optical thickness per retrieval window
raw_xch4	float	n	1e-9	Retrieved column dry-air mole fraction of atmospheric methane (XCH4) in ppb before bias correction
raw_xch4_err	float	n	1e-9	1-sigma statistical uncertainty of the retrieved column-average dry-air mole fraction of atmospheric methane
h2o_column	float	n	m-2	Retrieved total water column
surface_albedo_758	float	n		The retrieved albedo at 758 nm
surface_albedo_1593	float	n		The retrieved albedo at 1593 nm
surface_albedo_1629	float	n		The retrieved albedo at 1629 nm
surface_albedo_2042	float	n		The retrieved albedo at 2042 nm
intensity_offset_o2a	float	n	W cm-2	The retrieved intensity offset in the O2A band
aerosol_size	float	n		Retrieved size parameter of the aerosol distribution
aerosol_central_height	float	n	m	Peak height of the aerosol Gaussian height distribution
aerosol_total_column	float	n	m-2	Retrieved total aerosol column



1.3.2 Quality Flags and Metadata

There are quality flags "xco2_quality_flag" and "xch4_quality_flag" included in the data files. The quality flag can have 2 values:

- 0: retrieval quality has been checked
- 1: data should not be used (e.g., bad fit to data, residual cloud contamination)

For a GOSAT-2 ground pixel to be processed by the RemoTeC Full Physics algorithm it has to fulfill the following criteria: GOSAT-2 nominal quality flags should be good and the standard deviation of the elevation in the pixel should be less than 1000 meters (to filter out the most extreme terrains). After the retrieval step the data that fulfill the following criteria are flagged as '0' for land:

- Number of iteration steps in retrieval < 31.
- χ^2 of fit < 8
- SNR > 50
- Standard deviation of surface elevation within GOSAT-2 ground pixel should be < 100 m
- Aerosol Optical Thickness < 0.8
- $3 < \text{Aero_size} < 6$
- $\text{SZA} < 75^\circ$
- $0 < (2.4 * \text{albedo}[0.76 \text{ micron}]) - (1.13 * \text{albedo}[2.0 \text{ micron}]) < 0.8$
- $0 < \text{peak height of aerosol Gaussian height distribution} < 8000$
- $0 < \text{cirrus signal (2 micron)} < 2e-9$
- $0.99 < \text{CO}_2 (1.6 \text{ micron}) / \text{CO}_2 (2.0 \text{ micron}) < 1.018$
- $0.96 < \text{O}_2 (\text{retrieved}) / \text{O}_2 (\text{prior}) < 1.04$
- $0.95 < \text{H}_2\text{O} (1.6 \text{ micron}) / \text{H}_2\text{O} (2.0 \text{ micron}) < 1.08$

For sunglint:

- Number of iteration steps in retrieval < 31.
- χ^2 of fit < 8
- SNR > 50



- Standard deviation of surface elevation within GOSAT-2 ground pixel should be < 100 m
- $SZA < 75^\circ$
- $0 < (2.4 * \text{albedo}[0.76 \text{ micron}]) - (1.13 * \text{albedo}[2.0 \text{ micron}]) < 0.3$
- $0 < \text{cirrus signal} (2 \text{ micron}) < 2e-9$
- $0.99 < \text{CO}_2 (1.6 \text{ micron}) / \text{CO}_2 (2.0 \text{ micron}) < 1.003$
- $0.96 < \text{O}_2 (\text{retrieved}) / \text{O}_2 (\text{prior}) < 1.04$
- $0.95 < \text{H}_2\text{O} (1.6 \text{ micron}) / \text{H}_2\text{O} (2.0 \text{ micron}) < 1.08$

1.3.3 Recommended data usage

It is strongly recommended to only use the bias-corrected data in: "xco2" and "xch4" except if users explicitly correct for biases themselves (e.g., in an inverse modeling framework). Here, it should be noted that the bias correction has been developed independently for the different GOSAT-FTS-2 instrument settings (normal & sunglint).

Also, use only data over land (land type=0) except for sunglint cases.

If the data are to be compared with other XCO₂ and/or XCH₄ data for which vertical profile information is available (e.g., inverse modeling, comparison to models, comparison to measured profiles), the column averaging kernels should be used. Here it should be noted that the column averaging kernels are to be applied to layer sub-columns (m-2), as these are the quantities directly retrieved in the RemoTeC algorithm.

For model comparisons the retrieved XCO₂ should be compared to $[\text{VCO}_2]_{\text{model}} / [\text{VAIR}]_{\text{model}}$ where $[\text{VAIR}]_{\text{model}}$ is the total dry air column provided by the model and $[\text{VCO}_2]_{\text{model}}$ is the model total CO₂ column after applying the column averaging kernel, viz.:

$$[\text{VCO}_2]_{\text{model}}' = [\text{VCO}_2]_{\text{prior}} + a^T (x_{\text{model}} - x_{\text{prior}}) \quad (3)$$

Where $[\text{VCO}_2]_{\text{prior}}$ is the prior CO₂ total column used in the retrieval, x_{model} is the vertical CO₂ profile from the model (as sub-columns) and x_{prior} is the prior vertical profile from the retrieval. For application of the column averaging kernel the model vertical profile should be re-calculated on the vertical grid of the retrieval (preferred) or the averaging kernel has to be interpolated to the vertical grid of the model. This procedure holds in the same way for the SRFP XCH₄ product, but then replacing all instances of CO₂ with CH₄.



1.3.4 Tools for Reading the Data

The data are stored in Netcdf format which can be read with standard tools in the common programming languages (IDL, Matlab, Python, Fortran90, C++, etc). In python, several modules can be used to manipulate Netcdf files, such as netCDF4 (<https://pypi.org/project/netCDF4/>) , h5py (<https://docs.h5py.org/en/stable/>) and xarray (<https://docs.xarray.dev/en/stable/>). Netcdf functionality can also be implemented in compiled languages Fortran (<https://docs.unidata.ucar.edu/netcdf-fortran/current/>) and C++ (<http://unidata.github.io/netcdf-cxx4/index.html>).

1.3.5 Known Limitations and Issues

- The data retrieved for the normal observations are considered highest quality and are well validated. In the "raw" retrievals (i.e., before bias correction) there is a bias between normal and sunlint retrievals. Although these biases have been corrected in the bias-corrected products, there may still be a small residual bias left, especially due to the limited number of validation sites for sunlint retrievals.



2. 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:

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

Direct link to CH₄ products:

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

Tabs / riders lead to the following items:

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



References

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