ECMWF COPERNICUS REPORT

Copernicus Climate Change Service

Product User Guide and Specification (PUGS) – ANNEX C for product CH4_GO2_SRPR (v2.0.0, 2019-2021)

C3S2_312a_Lot2_DLR – Atmosphere

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

Date: 18/04/2023

Ref: C3S2_312a_Lot2_D-WP2_PUGS-2022-GHG_ANNEX-C_v6.3

Official reference number service contract: 2021/C3S2_312a_Lot2_DLR/SC1

PROGRAMME OF THE EUROPEAN UNION

IMPLEMENTED BY ECMWF

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: Some typos corrected and references added.	All
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 2nd 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	CH4_GO2_SRPR	CDR 6	2.0.0	31-Aug-2022

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 6 (2003-2021), project C3S2_312a_Lot2_DLR – Atmosphere, v6.3, 2023. *(this document is an ANNEX to the Main PUGS)*
D2	**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.
D3	Barr, A. G., et al., Algorithm Theoretical Basis Document (ATBD) – ANNEX C for product CH4 GO2 SRPR (v2.0.0, 2019-2021), Technical Report C3S project C3S2 312a Lot2 DLR – Atmosphere, version 6.2, 2023.

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., XCO_2) over one orbit
L3	Geophysical variables averaged in time and mapped on a global longitude/latitude horizontal grid
L4	Model output derived by assimilation of observations, or variables derived from multiple measurements (or both)

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Scope of document

This document is a Product User Guide and Specification (PUGS) for the Copernicus Climate Change Service (C3S, https://climate.copernicus.eu/) greenhouse gas (GHG) component as covered by project C3S2_312a_Lot2.

Within this project satellite-derived atmospheric carbon dioxide (CO_2) and methane (CH_4) 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 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 C3S2 product CH4_GO2_SRPR v2.0.0.

This product is the XCH_4 Level 2 product 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 CO_2 and CH_4, 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 (CO_2 and CH_4) 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 C of the Product User Guide (PUG), which is a deliverable of the C3S2 project. This document describes the XCH4 Proxy data products generated by the RemoTeC algorithm (CH4_GO2_SRPR). 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 how to use them. 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. Proxy Product

1.1 Data Product Description

The Japanese Greenhouse gases Observing SATellite-2 (GOSAT-2) was launched on 29th October 2018 and started operational observations form February 2019. GOSAT-2 provides dedicated global measurements of total column CO_2 and CH_4 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-C (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_SRPR product is retrieved from GOSAT-2 TANSO-FTS-2 NIR and SWIR spectra using the RemoTeC algorithm that has been 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 CO_2 bands at 1.61 and 2.06 µm, as well as a CH_4 band at 1.64 µm. Within the retrieval procedure the sub-columns of CO_2 and CH_4 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. As the Proxy* retrievals perform a non-scattering retrieval, the retrieved XCH4 column cannot be used directly, as effects of aerosol scattering modify the light path. To correct for this, in the PROXY approach, the retrieved XCH4 column is divided by the retrieved XCO2 column at the 1.61 µm band and then multiplied by a XCO2 total column. The retrieved XCH4 has been extensively validated with ground based TCCON measurements (Wunch et al. 2015). To further improve accuracy a bias correction has been developed based on TCCON comparisons. We use the GGG2020 release of the TCCON data.

*The Proxy product is so named since it approximates the impact of aerosols on the light path by assuming that CH_4 and CO_2 will be affected in the same way. By dividing the retrieved XCH4 by the retrieved XCO2, is is assumed that any aerosol induced errors due to the modification of the light path will be divided out. Thus XCO2 acts as a proxy for the presence of aerosols.

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

1.1.1 Bias Correction

From comparison with TCCON it was found that the error in XCH4 correlates with the retrieved albedo α at 1.6 um in band 2. Based on this correlation the following bias correction has been developed for XCH4:

$$XCH4_{corr} = XCH4 * (a + b * \alpha) \quad (1)$$

with a = 1.00196 , b = -0.00014 for normal (land) data, and a=1.00025 , b = -0.01221 for ocean (sunglint) 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.

Figure 2 shows global maps of XCH4 for land (normal) and ocean (sunglint) 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 XCH4 measurements for normal measurements.

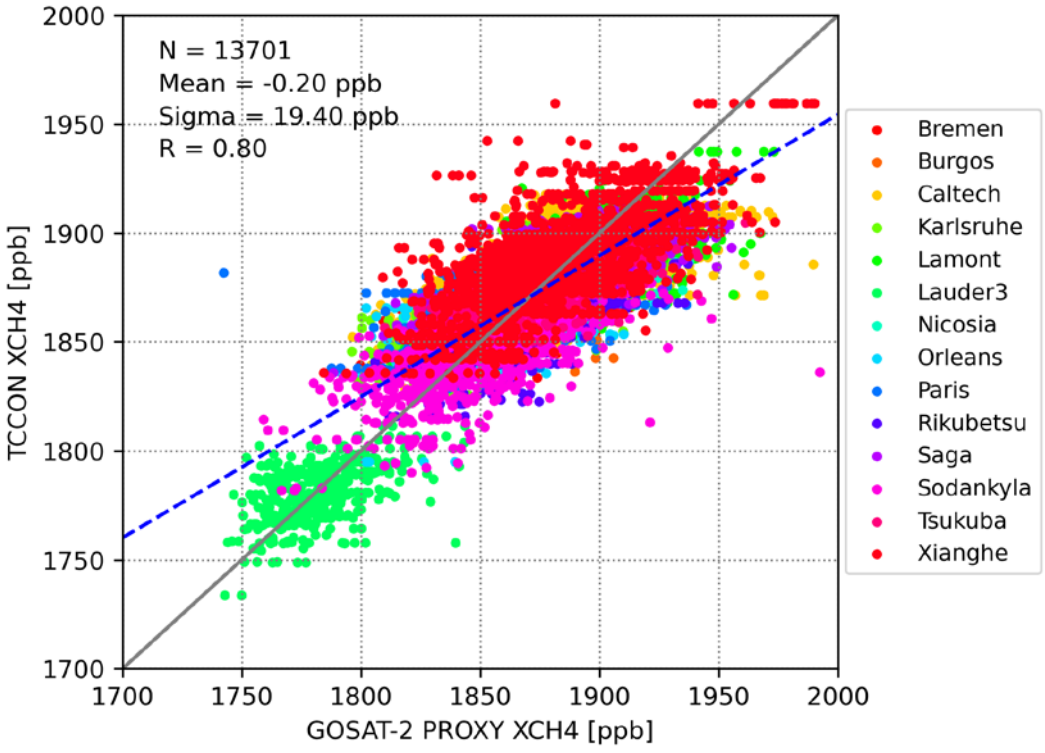
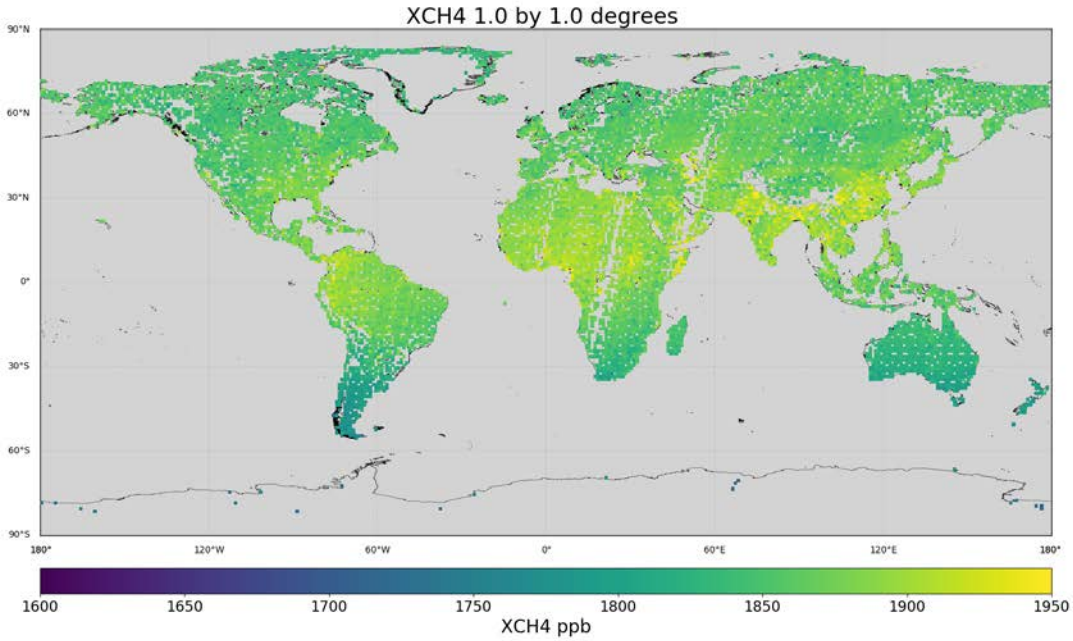
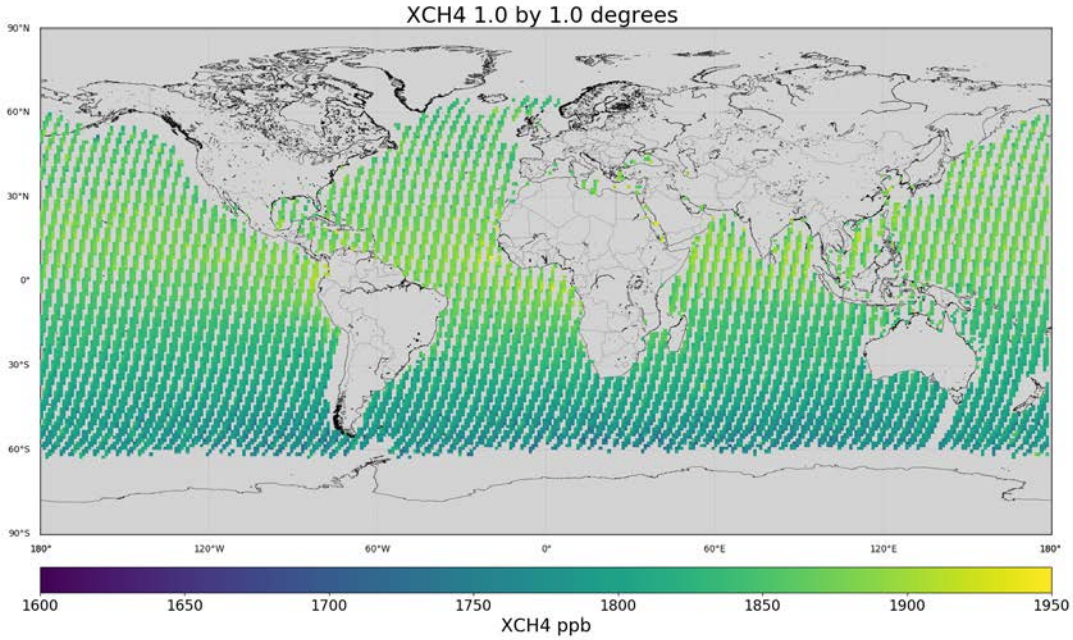


Figure 2: Global XCH4 for the 2019-2021 period for the CH4_GO2_SRPR product on a 1 by 1 degree resolution for both land (top) and sunglint (bottom) measurements.





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 are presented in Table 2. CO_2 and CH_4 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 CO_2 and CH_4, 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 (CO_2 and CH_4) 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: Target requirements for XCH4. (Threshold (T), Breakthrough (B) and Goal (G)) as derived in the Target Requirements Document (TRD) (*D2*).

Random and systematic error requirements for XCH4					
Parameter	**Req. type**	**Random error** ("Precision")		**Systematic error**	**Stability**
		Single obs.	1000^2 km^2 monthly		
XCH4	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 RemoTeC XCH4 data product v2.0.0 is 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 the key products, i.e. the retrieved column averaged dry air mixing ratio XCH4 with and without bias correction. Information relevant for the use of the data is included in the data file, like the vertical layering and averaging kernels. Also, the parameters that are retrieved simultaneously with XCH4 are included (e.g. surface albedo), as well as retrieval diagnostics like retrieval errors, and quality of the fit. Common and retrieval-specific variables for the XCH4 product are given in Tables 3 and 4, respectively.

Table 3: Common variables for the CH4_GO2_SRPR product v2.0.0.

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, 5	hPa	Pressure levels define boundaries of averaging kernel and mole fraction profile layers.
pressure_weight	float	n, 4		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, 4		Normalized column averaging kernel
ch4_profile_apriori	float	n, 4	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 4: Product specific (additional) variables for the CH4_GO2_SRPR product

Name	Type	Dim.	Units	Description
flag_landtype	int	n		0 = land, 1 = ocean
flag_sunglint	int	n		0 = no sunglint, 1 = sunglint
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, 4	m-2	Dry airmass per layer
altitude	float	n	m	Vertical altitude above the surface
air_temperature	float	n, 5	K	The bulk temperature of the air at each level
surface_altitude_stdv	float	n	m	Standard deviation of the surface elevation within the sounding
x_wind	float	n, 5	m s-1	Eastward wind velocity
y_wind	float	n, 5	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_err	float	n	1e-9	1-sigma statistical uncertainty of the retrieved column-average dry-air mole fraction of atmospheric methane
h2o_column_1593	float	n	m-2	Retrieved total water column at 1593 nm
h2o_column_1629	float	n	m-2	Retrieved total water column at 1629 nm
h2o_column_2042	float	n	m-2	Retrieved total water column at 2042 nm
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
raw_xch4	float	n	1e-9	Retrieved column dry-air mole fraction of atmospheric methane (XCH4) in ppb before scattering correction
xch4_no_bias_correction	float	n	1e-9	Retrieved column dry-air mole fraction of atmospheric methane (XCH4) in ppb before bias correction
raw_xco2	float	n	1e-6	Retrieved column dry-air mole fraction of atmospheric carbon dioxide (XCO2) in ppm before scattering correction
xco2_apriori	float	n	1e-6	A priori dry-air mole fraction of atmospheric carbon dioxide
co2_profile_apriori	float	n, 4	1e-6	A priori dry-air mole fraction profile of atmospheric carbon dioxide
xco2_averaging_kernel	float	n, 4		Normalized column averaging kernel for carbon dioxide
raw_xco2_err	float	n	1e-6	1-sigma statistical uncertainty of the retrieved column-average dry-air mole fraction of atmospheric carbon dioxide

1.3.2 Quality Flags and Metadata

There is a quality flag "xch4_quality_flag" included in the data file. 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 PROXY 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 terrain). After the retrieval the data that fulfill the following criteria are flagged as '0':

- Number of iteration steps in retrieval < 10.
- $\chi 2$ of fit < 18.
- SNR > 50.
- Standard deviation of surface elevation within GOSAT-2 ground pixel should be < 150 m
- SZA < 75^{o}.
- 0.98 < CO2 (1.6 micron) / CO2 (2.0 micron) < 1.08
- 0.91 < O2 (retrieved) / O2 (prior) < 1.05
- 0.92 < H2O (1.6 micron) / H2O (2.0 micron) < 1.25
- 0 < (2.4*albedo[0.76 micron]) – (1.13*albedo[2.0 micron]) < 0.8

1.3.3 Recommended data usage

It is strongly recommended to only use the bias-corrected data in: "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 (land & 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 $[VCO2]'_{model}/[VAIR]_{model}$ where

$[VAIR]_{model}$ is the total dry air column provided by the model and $[VCO2]'_{model}$ is the model total CO_2 column after applying the column averaging kernel, viz.:

$$[VCO2]'_{model} = [VCO2]_{prior} + a^T(x_{model} - x_{prior}) \quad (2)$$

where $[VCO2]_{prior}$ is the prior CO_2 total column used in the retrieval, x_{model} is the vertical CO_2 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.

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 sunglint 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 sunglint 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 CO_2 products:
https://cds.climate.copernicus.eu/cdsapp#!/dataset/satellite-carbon-dioxide?tab=overview

Direct link to CH_4 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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Copernicus Climate Change Service

ECMWF - Shinfield Park, Reading RG2 9AX, UK

Contact: https://support.ecmwf.int/