



Product User Guide and Specification (PUGS) – ANNEX A for products CO2_GOS_OCFP, CH4_GOS_OCFP (v7.3, 2009-2021) & CH4_GOS_OCPR (v9.0, 2009- 2021)

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 (2009-2016)	All
2.0	4-October-2018	Updated product description, filtering criteria, and bias correction information for v7.2 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: Only date and version number changed (for consistency reasons) as otherwise OK as is.	First few pages
4.0	18-August-2020	Update for CDR4 (2009-2019)	All
5.0	18-February-2021	Update for CDR5 (2009-mid2020)	All
6.0	04-August-2022	Update for CDR6 (2009-2021)	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_GOS_OCFP	CDR 6	7.3	31-Aug-2022
WP2-FDDP-GHG-v1	CH4_GOS_OCFP	CDR 6	7.3	31-Aug-2022
WP2-FDDP-GHG-v1	CH4_GOS_OCPR	CDR 6	9.0	31-Aug-2022



Related documents

Reference ID	Document
D1	<p>Main PUGS:</p> <p>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, 6.3, 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>



Acronyms

Acronym	Definition
AOD	Aerosol Optical Depth
CAR	Climate Assessment Report
C3S	Copernicus Climate Change Service
CCDAS	Carbon Cycle Data Assimilation System
ECMWF	European Centre for Medium Range Weather Forecasting
ECV	Essential Climate Variable
EU	European Union
FP	Full Physics retrieval method
FTS	Fourier Transform Spectrometer
GHG	GreenHouse Gas
GMES	Global Monitoring for Environment and Security
GOSAT	Greenhouse Gases Observing Satellite
GOSAT-2	Greenhouse Gases Observing Satellite 2
IUP	Institute of Environmental Physics (IUP) of the University of Bremen, Germany
JAXA	Japan Aerospace Exploration Agency
L1	Level 1
L2	Level 2
L3	Level 3
L4	Level 4
LMD	Laboratoire de Météorologie Dynamique
LMDZ	Laboratoire de Météorologie Dynamique Zoom (Global climate model)
MACC	Monitoring Atmospheric Composition and Climate, EU GMES project
NA	Not applicable
NetCDF	Network Common Data Format
NIR	Near Infra Red
NOAA	National Oceanic and Atmospheric Administration
OCO	Orbiting Carbon Observatory
OE	Optimal Estimation
PCA	Principal Component Analysis
ppb	Parts per billion
ppm	Parts per million
PR	(light path) PROxy retrieval method
PQAR	Product Quality Assessment Report
RANSAC	RANdom Sample Consensus
SNR	Signal-to-Noise Ratio
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
TCCON	Total Carbon Column Observing Network
TIR	Thermal Infra Red
TR	Target Requirements
TRD	Target Requirements Document
UoL	University of Leicester, United Kingdom



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)



Table of Contents

History of modifications	4
List of datasets covered by this document	5
Related documents	6
Acronyms	7
General definitions	9
Scope of document	11
Executive summary	12
1 Product description	13
1.1 The GOSAT-FTS Instrument	13
1.2 The University of Leicester Products	13
1.3 Post-retrieval processing	18
1.3.1 Filtering	18
1.3.2 Pre-retrieval screening	18
1.3.3 Post-retrieval screening	18
1.3.4 Bias correction	21
2 Target requirements	23
3 Data usage information	25
3.1 Tools for reading the data	25
3.2 Known limitations and issues	25
3.3 Data file content	25
4 Data access information	33
12 References	34



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 (CO₂) and methane (CH₄) Essential Climate Variable (ECV) data products will be 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 C3S products CO2_GOS_OCFP (v7.3), CH4_GOS_OCFP (v7.3) and CH4_GOS_OCPR (v9.0).

These products are XCO₂ and XCH₄ Level 2 products as retrieved from GOSAT using algorithms developed at the University of Leicester, UK.



Executive summary

This document summarises the data and metadata stored in the Copernicus Climate Change Service (C3S) Level 2 CO₂ and CH₄ data products developed by the University of Leicester (UoL). These products provide the column-averaged dry-air mixing ratios (mole fractions) of CO₂ (XCO₂) and (XCH₄), derived from short-wave infrared (SWIR) spectra from the JAXA Greenhouse gases Observing SATellite (GOSAT). The datasets discussed in this work cover the entire satellite operational period (2009-2021), and are published as daily netCDF files available from the C3S website: <https://climate.copernicus.eu/>.

The aim of this document is to describe to users the quality flags and metadata, data format, product grid and geographical projection, known limitations, and available tools for decoding and interpreting the data. In addition, this document also briefly discusses the validation of these datasets against the C3S target requirements stated in TRD GHG, 2017 (see related documents). This is done through comparisons with highly accurate ground-based measurements provided by the Total Carbon Column Observing Network (TCCON). This ensures that we have confidence that the datasets in this work at least meet the breakthrough requirements set in the TRD. Overall, the UoL datasets meet the stringent precision and accuracy requirements set by C3S, and are believed to offer information on regional surface fluxes of CO₂ and CH₄.



1 Product description

1.1 The GOSAT-FTS Instrument

The Japanese Greenhouse gases Observing SATellite (GOSAT) was launched on 23rd January 2009, Yokota et al., 2009, by JAXA, the Japanese Space Agency. GOSAT provides the first dedicated global measurements of total column CO₂ and CH₄ from its SWIR bands, Yoshida et al., 2013. It is equipped with two instruments; the Thermal And Near-infrared Sensor for carbon Observations - Fourier Transform Spectrometer (TANSO-FTS), and a dedicated Cloud and Aerosol Imager (TANSO-CAI). A more detailed description can be found in the ATBD, Boesch et al., 2019.

1.2 The University of Leicester Products

The UoL have generated three greenhouse gas datasets from GOSAT TANSO-FTS NIR and SWIR spectra, which are discussed in this section:

XCO₂:

- CO2_GOS_OCFP (v 7.3)

XCH₄:

- CH4_GOS_OCFP (v 7.3)
- CH4_GOS_OCPR (v 9.0)

All products mentioned in this document are retrieved using the University of Leicester (UoL) Full-Physics Retrieval Algorithm, based on the original Orbiting Carbon Observatory (OCO) Full Physics retrieval algorithm, modified for use with GOSAT spectra (OCFP).

The retrieval algorithm uses an iterative retrieval scheme based on Bayesian optimal estimation to retrieve a set of atmospheric, surface and instrument parameters, referred to as the state vector, from measured spectral radiances, Boesch et al., 2011; Connor et al., 2008. The forward model, used to relate the state vector to the measured radiances, includes the LIDORT, Spurr, 2008, and TWOSTR, Spurr et al., 2011, radiative transfer models combined with a fast 2 orders of scattering vector radiative transfer code, Natraj et al., 2008. In order to accelerate the radiative transfer component of the retrieval algorithm, the code uses the low stream interpolation (LSI) method described in O'Dell, 2010, or the principal component analysis (PCA)-based fast RT scheme described in Somkuti et al., 2017.

In addition to the Full-Physics retrieval products, we also offer a separate product for CH₄, which is retrieved using the Full-Physics algorithm modified by the “proxy” technique (OCPR) as discussed in Parker et al., 2011, Parker et al., 2015 and Parker et al., 2020. CO₂ is known to vary in the atmosphere much less than CH₄ and as the CO₂ absorption band is spectrally close to that of CH₄ we can use the CO₂ as a proxy for the light path to minimize common spectral artefacts due to aerosol scattering and instrumental effect. CH₄ and CO₂ retrievals are carried out sequentially with channels at 1.65 μm and 1.61 μm respectively.



In order to obtain a volume mixing ratio (VMR) of CH_4 , it is necessary to multiply the retrieved $\text{XCH}_4/\text{XCO}_2$ ratio by a model XCO_2 . We obtain the CO_2 VMRs from the median of a model CO_2 ensemble that comprises GEOS-Chem (University of Edinburgh), LMDZ/MACC-II and NOAA CarbonTracker, convolved with scene-dependent instrument averaging kernels obtained from the GOSAT $1.6 \mu\text{m}$ CO_2 retrieval.

Figures 1-3 show the global seasonal variation of XCO_2 and XCH_4 over all three data products between April 2009 and December 2021.



Figure 1: Global seasonal maps of UoL GOSAT XCO₂ (CO₂_GOS_OCFP) retrieved between April 2009 and December 2021.

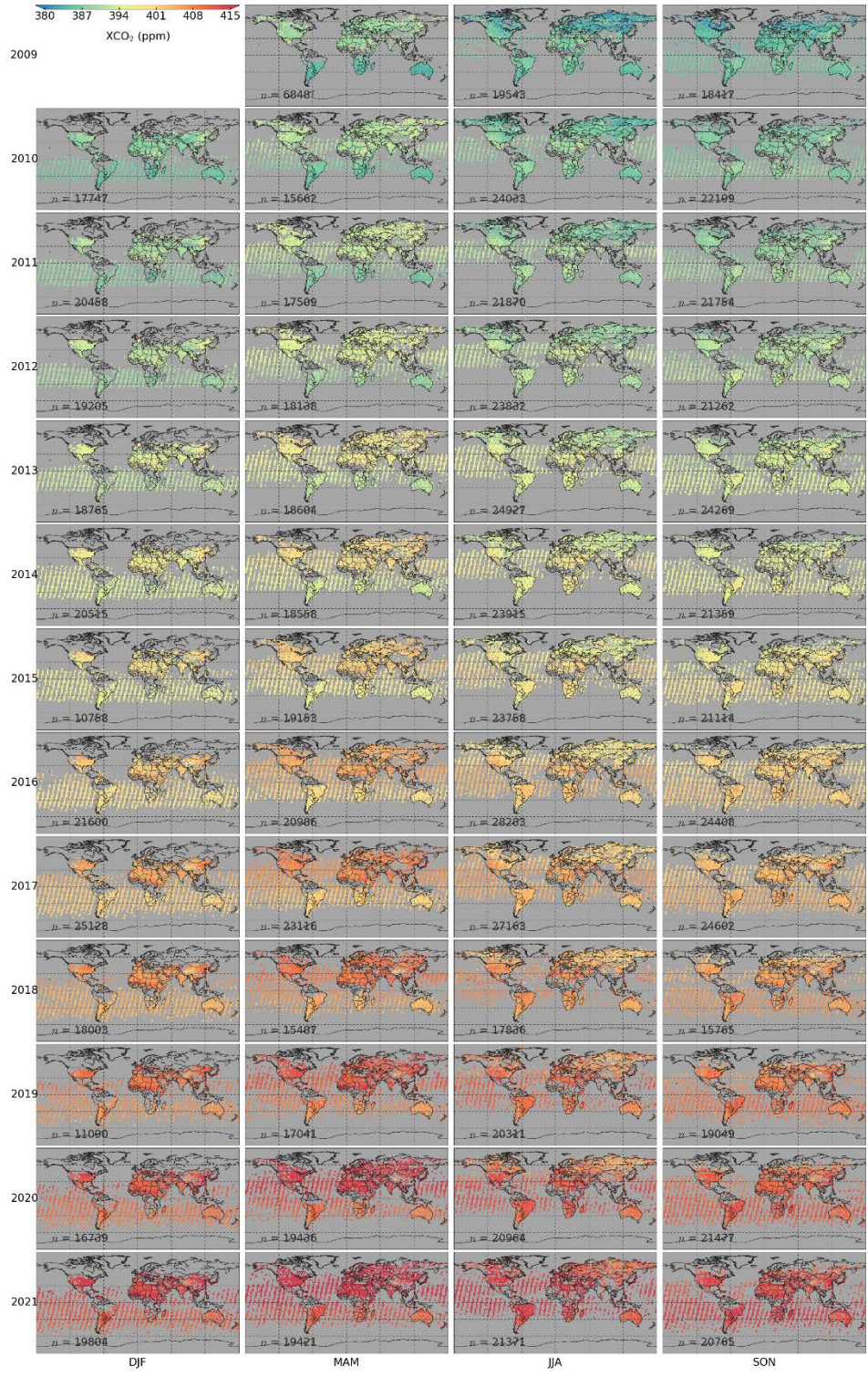




Figure 2: Global seasonal maps of UoL GOSAT XCH₄ (CH₄_GOS_OCFP) retrieved between April 2009 and December 2021.

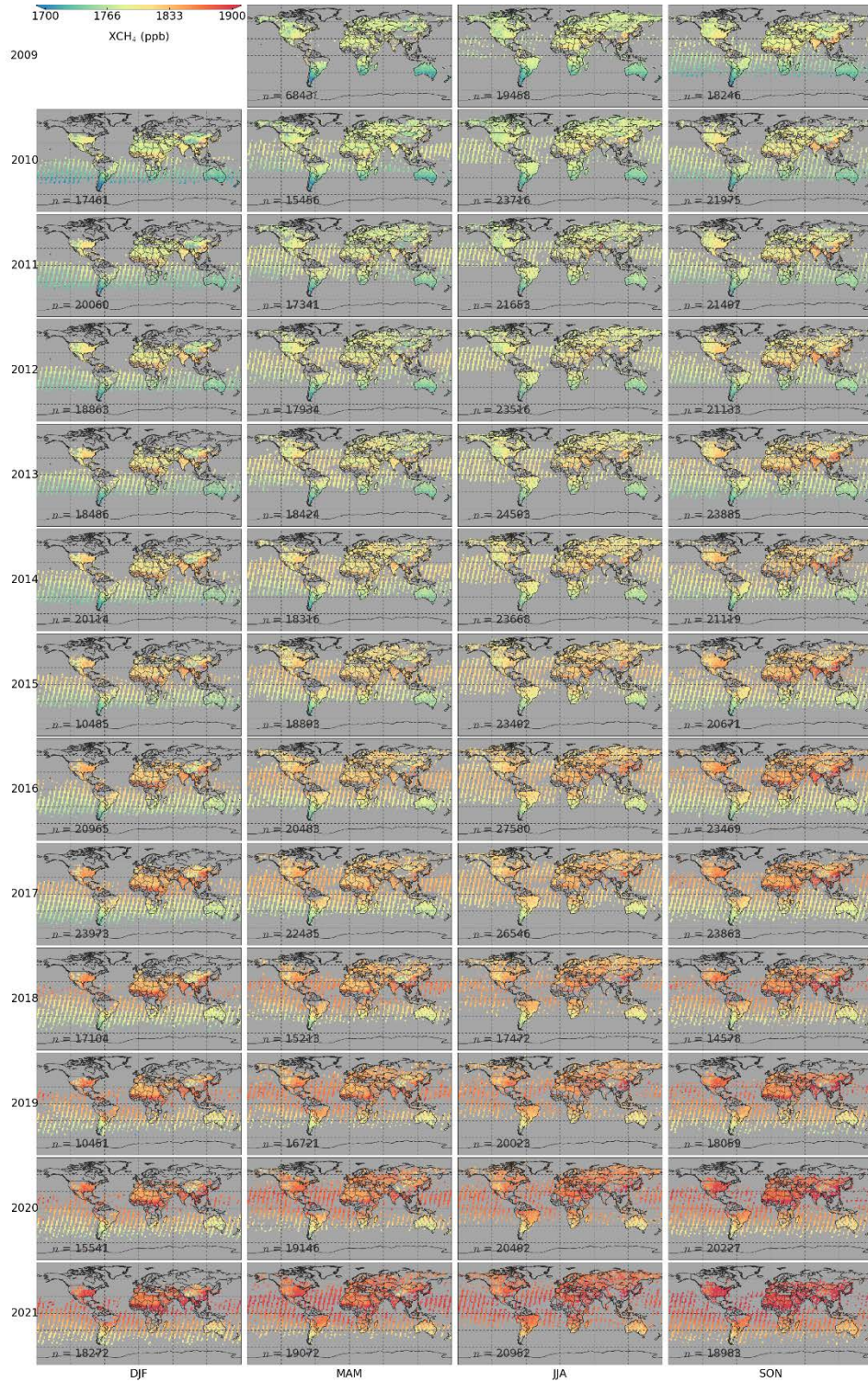
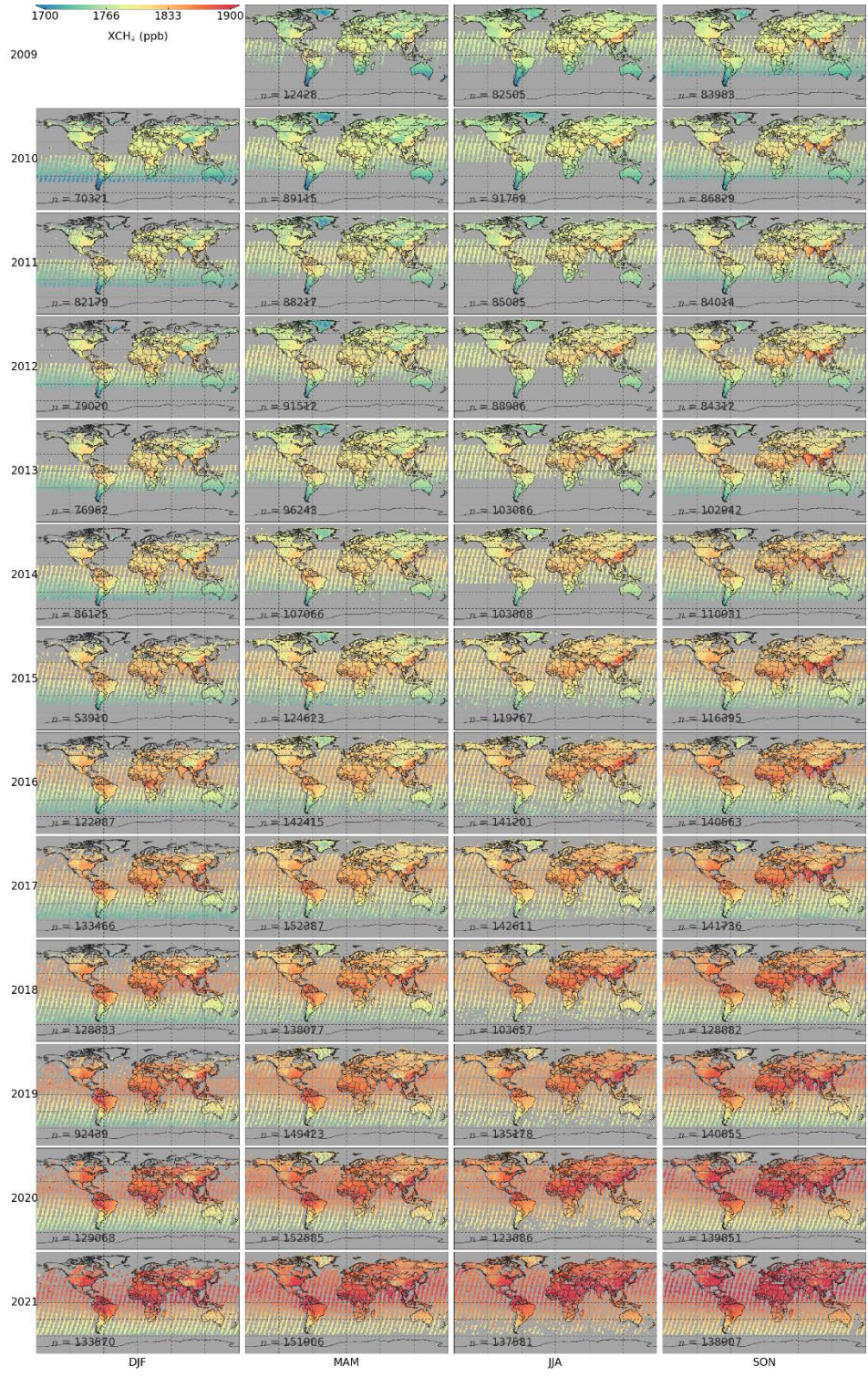




Figure 3: Global seasonal maps of UoL GOSAT XCH₄ (CH₄_GOS_OCPR) retrieved between April 2009 and December 2021.





1.3 Post-retrieval processing

1.3.1 Filtering

To ensure data quality, the GOSAT data is filtered for anomalously high or low retrieval fit statistics, along with anomalous values in its geophysical or final state vector parameters. The filtering criteria were empirically determined through analysis of the fit statistics, along with comparisons made with co-located ground-based measurements from the Total Carbon Column Observing Network (TCCON, See Section 2).

1.3.2 Pre-retrieval screening

Before a retrieval is performed, the GOSAT soundings are subjected to several tests for measurement noise and other issues. For CO₂_GOS_OCFP and CH₄_GOS_OCFP, only soundings that pass the criteria shown in Table 2 are used in the retrieval. For the CH₄_GOS_OCPR product, only the cloud screening and geographic criteria shown in Table 2 are applied.

Table 2: The pre-retrieval filtering criteria used in the CO₂_GOS_OCFP and CH₄_GOS_OCFP products.

Parameter	Filtering criteria
SNR (all bands)	≥ 20
SZA	$\leq 75^\circ$
Latitude	$\geq 60^\circ$ S
Δ (Surface pressure): difference between retrieved and a priori value (cloud screen)	≤ 30 hPa
Weak/strong CO ₂ column ratio	$\geq 0.98, \leq 1.05$

1.3.3 Post-retrieval screening

After the retrieval, the datasets are subsequently screened to determine if the retrieval was successful. Data retrieved from glint and land measurements are filtered separately, as viewing conditions are markedly different over oceans. The post-filtering criteria used in the CO₂_GOS_OCFP are shown in Table 3. For CH₄_GOS_OCFP only soundings, which had previously passed the CO₂_GOS_OCFP filtering were considered useful. The CH₄ retrievals from these soundings were then subsequently filtered again using the criteria shown in Table 4 before being flagged as good data. Retrievals from 2018 onwards use a new version of GOSAT L1B data (V210.210 instead of V201.202, Kataoka et al., 2019).



Table 3: The post-retrieval filtering criteria used in the CO2_GOS_OCFP product.

Parameter	Filtering criteria	
	Land	Glint
Retrieval outcome	Converged	Converged
SNR (all bands)	≥ 45	≥ 45
n retrieval iterations	≤ 7	≤ 7
SZA	$\leq 65^\circ$	NA
n diverging retrieval steps	≤ 2	≤ 2
χ^2 (Band 1)	$\geq 0.5, \leq 1.55$	$\geq 0.9, \leq 1.45$
χ^2 (Band 2)	$\geq 0.6, \leq 2.0$	$\geq 0.8, \leq 1.70$
χ^2 (Band 3)	$\geq 0.5, \leq 1.55$	$\geq 0.65, \leq 1.25$
Weak/strong CO ₂ column ratio	$\geq 0.99, \leq 1.01$	$\geq 0.99, \leq 1.01$
XCO ₂ a posteriori error	≤ 2.5 ppm	≤ 1.15 ppm
Total AOD (cirrus + small + large aerosols)	≤ 0.5	≤ 0.17
AOD (small aerosol)	≤ 0.3	≤ 0.3
AOD (large aerosol)	≤ 0.15	≤ 0.08
Δ AOD (large aerosol): difference between retrieved and a priori value	≥ -1.8	≥ -1.25
Δ AOD (cirrus): difference between retrieved and a priori value	≥ -6.25	≥ -7.0
σ surface pressure within ground pixel	≤ 20 hPa	NA
Δ (Surface pressure): difference between retrieved and a priori value (cloud screen)	NA	$\geq -3.32, \leq 1.0$
Albedo slope (Band 1)	$\leq 2.5 \times 10^{-5}$	$\geq 2.6 \times 10^{-6}, \leq 1.75 \times 10^{-5}$
Albedo slope (Band 2)	NA	$\geq 0.0, \leq 5.0 \times 10^{-6}$
Albedo slope (Band 3)	$\geq -2.0 \times 10^{-4}$	$\geq 0.0, \leq 2.5 \times 10^{-5}$
Albedo ratio between band 1 and band 2	≤ 2.75	$\geq 0.98, \leq 1.2$
Albedo ratio between band 1 and band 3	NA	$\geq 1.09, \leq 1.2$
Retrieved CO ₂ profile gradient between the surface and retrieval level 15	NA	$\geq 0.9, \leq 1.01$



The soundings, which pass the filtering criteria in the CO2_GOS_OCFP product, are subsequently filtered again using the criteria in Table 4 to provide filtered data for CH4_GOS_OCFP.

Table 4: The post-retrieval filtering criteria used in the CH4_GOS_OCFP product. Note that soundings are first filtered using the XCO₂ retrieval parameters shown in Table 3. Each parameter indicates whether the considered value is taken from the XCO₂ or XCH₄ retrieval.

Parameter	Filtering criteria	
	Land	Glint
Retrieval outcome (XCH ₄)	Converged	Converged
SNR (all bands)	≥ 45	≥ 45
<i>n</i> retrieval iterations (XCH ₄)	≤ 7	≤ 7
<i>n</i> diverging retrieval steps (XCH ₄)	≤ 2	≤ 2
χ ² (Band 2, XCH ₄)	≤ 3.6	≥ 0.86, ≤ 1.44
Albedo slope (Band 2, XCH ₄)	≥ -5.5 × 10 ⁻⁵	NA
XCH ₄ a posteriori error	≤ 9.5 ppb	NA
σ surface pressure within ground pixel (XCO ₂)	NA	≤ 2.38 hPa

Table 5: The post-retrieval filtering criteria used in the CH4_GOS_OCPR product.

Parameter	Filtering criteria
χ ² (XCH ₄ retrieval)	≥ 0.4, ≤ 1.9
χ ² (XCO ₂ retrieval)	≥ 0.4, ≤ 1.9
XCH ₄ a posteriori error	≤ 20 ppb
XCO ₂ a posteriori error	≤ 3 ppm
Retrieved XCH ₄	≥ 1650 ppb
Retrieved XCO ₂	≥ 350 ppm



1.3.4 Bias correction

For these data products, a bias correction based on several state vector parameters is calculated via a regression analysis of the difference between collocated GOSAT and TCCON XCH₄ and XCO₂ observations. Land and glint measurements were corrected separately for each product.

For CO₂_GOS_OCFP and CH₄_GOS_OCFP, the correction takes the form of a linear equation of n state vector parameters (\mathbf{x}) multiplied by a unique coefficient (m) along with a single offset (c), such that:

$$\text{correction} = c + m_0x_0 + m_1x_1 + \dots + m_{n-1}x_{n-1} \quad (1)$$

The correction is then subtracted from the original XCO₂ or XCH₄ to give the final value:

$$\text{XCO}_{2\text{final}} = \text{XCO}_2 - \text{correction} \quad (2)$$

The regression analysis makes use of the RANSAC method (Fischler and Bolles, 1981) to avoid statistical outliers affecting the fit. As such, the total mean bias against TCCON remaining in the data after this correction is not zero (see Section 2).

Tables 6-9 show the values of m and c used to correct the land and glint data in the CO₂_GOS_OCFP and CH₄_GOS_OCFP products.



Table 6: The parameters and coefficient values used in the bias correction for the CO₂_GOS_OCFP product (land soundings only). As part of the bias correction, an additive offset of -17.96 ppm is also applied, which has resulted in the best fit to the TCCON reference data.

Parameter	Coefficient
Retrieved CO ₂ profile gradient between the surface and retrieval level 15	19.75
AOD (large aerosol)	-25.57

Table 7: The parameters and coefficient values used in the bias correction for the CO₂_GOS_OCFP product (glint soundings only). An offset of: -23.44 ppm is also applied.

Parameter	Coefficient
Albedo slope (Band 3)	1.39×10^5
Retrieved CO ₂ profile gradient between the surface and retrieval level 15	24.80
Total AOD (cirrus + small + large aerosols)	-13.20
Albedo slope (Band 1)	-4.01×10^4

Table 8: The parameters and coefficient values used in the bias correction for the CH₄_GOS_OCFP product (land soundings only). An offset of: -0.125 ppb is also applied. Each parameter indicates whether the considered value is taken from the XCO₂ or XCH₄ retrieval.

Parameter	Coefficient
Albedo ratio between band 1 and band 3 (XCO ₂)	4.58
Total AOD (cirrus + small + large aerosols, XCO ₂)	-68.35
Albedo slope (Band 2, XCO ₂)	1.25×10^5

Table 9: The parameters and coefficient values used in the bias correction for the CH₄_GOS_OCFP product (glint soundings only). An offset of: 10.79 ppb is also applied. Each parameter indicates whether the considered value is taken from the XCO₂ or XCH₄ retrieval.

Parameter	Coefficient
Total AOD (cirrus + small + large aerosols, XCO ₂)	-89.77
Albedo slope (Band 1, XCO ₂)	-1.44×10^6

For CH₄_GOS_OCPR a simple global bias correction of -7.71 ppb is applied to all data to remove the mean bias to TCCON.



2 Target requirements

Products submitted to C3S must fulfill a number of stringent quality requirements, which are further discussed in the Target Requirements Document; TRD GHG, 2017. A full summary of these requirements, and how far our products fulfil them, is available in the PQAR Document. In this section we briefly summarise the requirements for random and systematic errors, and validate our products using TCCON data. Table 10 shows the random and systematic errors stated in the TRD.

Table 10: XCO₂ and XCH₄ random (“precision”) and systematic retrieval error requirements for measurements over land. Abbreviations: G:Goal, B:Breakthrough, T:Threshold requirement. §) Required systematic error after an empirical bias correction, that does not use the verification data. #) Required systematic error and stability after bias correction, where bias correction is not limited to the application of a constant offset / scaling factor.

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 #)

For both full-physics products, we have considered the land and glint measurements separately (see PQAR Document). Table 11 shows a summary of the statistics generated from direct comparisons between GOSAT and TCCON. The mean GOSAT-TCCON bias is a representation of the true systematic error, while the standard deviation is a representation of the true random error. Therefore, all datasets achieve at least the breakthrough requirements for XCO₂ and XCH₄ stated in Table 10.



Table 11: The results of direct comparisons between the UoL products and TCCON for GOSAT soundings between April 2009 and December 2017.

Dataset	Number of measurements	Pearson coefficient (r)	Mean bias	Standard deviation
XCO ₂ (land)	21965	0.96	0.00 ppm	1.85 ppm
XCO ₂ (glint)	1255	0.97	0.24 ppm	1.19 ppm
XCH ₄ (OCFP, land)	21863	0.91	-0.31 ppb	13.94 ppb
XCH ₄ (OCFP, glint)	1189	0.92	0.40 ppb	10.05 ppb
XCH ₄ (OCPR, land)	64454	0.92	-1.25 ppb	13.81 ppb
XCH ₄ (OCPR, glint)	8060	0.92	3.80 ppb	12.35 ppb



3 Data usage information

3.1 Tools for reading the data

The datasets are stored in netCDF4 format, which can be read with standard tools in common programming languages such as Python, Matlab, IDL and R.

3.2 Known limitations and issues

Users must be aware of the following caveats when using these datasets:

- As discussed in Section 1.3.2 we apply a bias correction to the data based on linear regression of geophysical parameters against the observed GOSAT-TCCON bias.
- A preliminary comparison of our XCO_2 and XCH_4 a posteriori errors against the standard deviation of the GOSAT-TCCON differences has indicated that our error estimates are potentially too small. For the `xco2_uncertainty` reported in the `CO2_GOS_OCFP` data product, we have multiplied the a posteriori error by a factor of 1.75 for land observations and 1.17 for glint observations so that it is a more realistic value. Similarly, the `xch4_uncertainty` reported in the `CH4_GOS_OCFP` product has been multiplied by a factor of 1.73 for land observations and 1.23 for glint observations. Further exploration of this will be performed as part of the validation exercises.
- For the `CH4_GOS_OCPR` product, more information about the models used to estimate the true XCO_2 column can be found in Section 1.2. If you wish to renormalize the XCH_4/XCO_2 ratio with your own model XCO_2 data, please be aware that you should first apply the provided averaging kernels to your model data.

3.3 Data file content

netCDF data files contain all of the common parameters for the C3S data products, as well as additional product-specific parameters. The dimension n refers to the number of retrievals in a given file, whilst the dimension m refers to the number of levels at which CO_2 and CH_4 profiles are retrieved. For `CO2_GOS_OCFP`, `CH4_GOS_OCFP` and `CH4_GOS_OCPR` data products m is set to 20. For some soundings made over high terrain in `CH4_GOS_OCPR` the lowest level is removed to ensure that all levels used to compute XCH_4 and XCO_2 are above the surface. In this case, values in the 20th level are replaced with the fill value -9999.99. Users reading averaging kernel and pressure level information will always see 20 levels, but will need to check whether the lowest level has been replaced with the fill value.



Table 12: Variables present in the CO2_GOS_OCFP product.

Name	Type	Dimensions	Units	Description
solar_zenith_angle	float	n	degree	Angle between line of sight to the sun and local vertical
sensor_zenith_angle	float	n	degree	Angle between the line of sight to the sensor and the local vertical
time	double	n	seconds since 1970-01-01 00:00:00	Measurement time
longitude	float	n	degrees_east	Centre longitude
latitude	float	n	degrees_north	Centre latitude
pressure_levels	float	n, m	hPa	Vertical altitude coordinate in pressure units as used for averaging kernels
pressure_weight	float	n, m		Pressure weights as used for averaging kernels
xco2	float	n	1e-6	Retrieved column-averaged dry-air mole fraction of atmospheric carbon dioxide (XCO ₂) in ppm.
xco2_no_bias_correction	float	n	1e-6	Retrieved column-averaged dry-air mole fraction of atmospheric carbon dioxide (XCO ₂) in ppm. No bias correction is applied
xco2_uncertainty	float	n	1e-6	Statistical uncertainty of XCO ₂ in ppm (1 σ)
xco2_averaging_kernel	float	n, m		XCO ₂ averaging kernel (a profile = vector for each single observation). Quantifies the altitude sensitivity of the XCO ₂ retrieval
co2_profile_apriori	float	n, m	1e-6	A-priori mole fraction profile of atmospheric CO ₂ in ppm
exposure_id	char	n, 22		Exposure identification number of the sounding
surface_altitude	float	n	metres	Altitude is the (geometric) height above the geoid, which is the reference geopotential surface
surface_altitude_stdev	float	n	metres	Standard deviation of the surface elevation within the area of the GOSAT sounding,



				as derived from the SRTM database
surface_air_pressure_apriori	float	n	hPa	A-priori surface pressure value
surface_air_pressure_apriori_std	float	n	hPa	A-priori surface pressure standard deviation
gain	byte	n		GOSAT TANSO-FTS instrument gain mode. 1 indicates high gain. 0 indicates medium gain
air_temperature_apriori	float	n, m	K	Air temperature is the bulk temperature of the air, not the surface (skin) temperature
h2o_profile_apriori	float	n, m	ppm	A-priori mole fraction profile of atmospheric H ₂ O in ppm
total_aod	float	n		Retrieved total aerosol optical depth
aod_type1	float	n		Retrieved AOD (small)
aod_type2	float	n		Retrieved AOD (large)
cirrus	float	n		Retrieved AOD (cirrus)
retr_flag	byte	n		Retrieval type flag (0 = land, 1 = glint)



Table 13: Variables present in the CH4_GOS_OCFP product

Name	Type	Dimensions	Units	Description
solar_zenith_angle	float	n	degree	Angle between line of sight to the sun and local vertical
sensor_zenith_angle	float	n	degree	Angle between the line of sight to the sensor and the local vertical
time	double	n	seconds since 1970-01-01 00:00:00	Measurement time
longitude	float	n	degrees_east	Centre longitude
latitude	float	n	degrees_north	Centre latitude
pressure_levels	float	n, m	hPa	Vertical altitude coordinate in pressure units as used for averaging kernels
pressure_weight	float	n, m		Pressure weights as used for averaging kernels
xch4	float	n	1e-9	Retrieved column-averaged dry-air mole fraction of atmospheric methane (XCH ₄) in ppb
xch4_no_bias_correction	float	n	1e-9	Retrieved column-averaged dry-air mole fraction of atmospheric methane (XCH ₄) in ppb. No bias correction is applied
xch4_uncertainty	float	n	1e-9	Statistical uncertainty of XCH ₄ in ppb (1 σ)
xch4_averaging_kernel	float	n, m		XCH ₄ averaging kernel (a profile = vector for each single observation). Quantifies the altitude sensitivity of the XCH ₄ retrieval
co2_profile_apriori	float	n, m	1e-6	A-priori mole fraction profile of atmospheric CO ₂ in ppm
ch4_profile_apriori	float	n, m	1e-9	A-priori mole fraction profile of atmospheric CH ₄ in ppb
exposure_id	char	n, 22		Exposure identification number of the sounding
surface_altitude	float	n	metres	Altitude is the (geometric) height above the geoid, which is the reference geopotential surface
surface_altitude_stdev	float	n	metres	Standard deviation of the surface elevation within the



				area of the GOSAT sounding, as derived from the SRTM database
surface_air_pressure_apriori	float	n	hPa	A-priori surface pressure value
surface_air_pressure_apriori_std	float	n	hPa	A-priori surface pressure standard deviation
gain	byte	n		GOSAT TANSO-FTS instrument gain mode. 1 indicates high gain. 0 indicates medium gain
air_temperature_apriori	float	n, m	K	Air temperature is the bulk temperature of the air, not the surface (skin) temperature
h2o_profile_apriori	float	n, m	ppm	A-priori mole fraction profile of atmospheric H ₂ O in ppm
total_aod	float	n		Retrieved total aerosol optical depth
aod_type1	float	n		Retrieved AOD (small)
aod_type2	float	n		Retrieved AOD (large)
cirrus	float	n		Retrieved AOD (cirrus)
retr_flag	byte	n		Retrieval type flag (0 = land, 1 = glint)



Table 14: Variables present in the CH4_GOS_OCPR product.

Name	Type	Dimensions	Units	Description
solar_zenith_angle	float	n	degree	Angle between line of sight to the sun and local vertical
sensor_zenith_angle	float	n	degree	Angle between the line of sight to the sensor and the local vertical
time	double	n	seconds since 1970-01-01 00:00:00	Measurement time
longitude	float	n	degrees_east	Centre longitude
latitude	float	n	degrees_north	Centre latitude
pressure_levels	float	n, m	hPa	Vertical altitude coordinate in pressure units as used for averaging kernels
pressure_weight	float	n, m		Pressure weights as used for averaging kernels
xch4	float	n	1e-9	Retrieved column-averaged dry-air mole fraction of atmospheric methane (XCH ₄) in ppb.
xch4_uncertainty	float	n	1e-9	Statistical uncertainty of XCH ₄ in ppb (1 σ)
xch4_averaging_kernel	float	n, m		XCH ₄ averaging kernel (a profile = vector for each single observation). Quantifies the altitude sensitivity of the XCH ₄ retrieval
co2_profile_apriori	float	n, m	1e-6	A-priori mole fraction profile of atmospheric CO ₂ in ppm
ch4_profile_apriori	float	n, m	1e-9	A-priori mole fraction profile of atmospheric CH ₄ in ppb
raw_xco2	float	n	ppm	Retrieved 1.6 μ m XCO ₂
raw_xch4	float	n	ppb	Retrieved 1.6 μ m XCH ₄
raw_xco2_error	float	n	ppm	Retrieved 1.6 μ m XCO ₂ error
raw_xch4_error	float	n	ppb	Retrieved 1.6 μ m XCH ₄ error
model_xco2	float	n	ppm	Model XCO ₂ component of the final proxy data product
model_xco2_range	float	n	ppm	Maximum difference (in ppm) between model XCO ₂ from GEOS-Chem, CarbonTracker and LMDZ
exposure_id	char	n, 22		Exposure identification number of the sounding



surface_altitude	float	n	metres	Altitude is the (geometric) height above the geoid, which is the reference geopotential surface
surface_altitude_stdev	float	n	metres	Standard deviation of the surface elevation within the area of the GOSAT sounding, as derived from the SRTM database
surface_air_pressure_apriori	float	n	hPa	A-priori surface pressure value
surface_air_pressure_apriori_std	float	n	hPa	A-priori surface pressure standard deviation
gain	byte	n		GOSAT TANSO-FTS instrument gain mode. 1 indicates high gain. 0 indicates medium gain
air_temperature_apriori	float	n, m	K	Air temperature is the bulk temperature of the air, not the surface (skin) temperature
h2o_profile_apriori	float	n, m	ppm	A-priori mole fraction profile of atmospheric H ₂ O in ppm
total_aod	float	n		Retrieved total aerosol optical depth
aod_type1	float	n		Retrieved AOD (small)
aod_type2	float	n		Retrieved AOD (large)
cirrus	float	n		Retrieved AOD (cirrus)
retr_flag	byte	n		Retrieval type flag (0 = land, 1 = glint)



For all data products, the `xco2_quality_flag` or `xch4_quality_flag` variable must be applied to the data (section 3.3) before use; a value of 0 indicates that the data has passed our quality control. These flags are given in the data products. Details how these flags are inferred are given in section 1.3. All vertically resolved data is provided on levels (as opposed to layers). This is especially important when applying UoL averaging kernels to model data.

For the `CO2_GOS_OCFP` and `CH4_GOS_OCFP` products, most users will be interested in the `xch4` or `xco2` variables, which store the column-averaged dry-air mixing ratios of the required gas. We also provide the values of the mixing ratios before any bias correction is applied, which are stored in the `xco2_no_bias_correction/xch4_no_bias_correction` variable.

For `CH4_GOS_OCPR`, the final proxy data product is stored in the `xch4` variable. It is recommended that users use this variable unless explicitly interested in the retrieved XCH_4/XCO_2 ratio. Users interested in the raw XCH_4 and XCO_2 retrieved from the 1.6 μm band uncorrected for aerosol scattering can find these values stored in the `raw_xch4` and `raw_xco2` variables.

We also include other important variables, such as averaging kernels, errors, and geolocation data in the netCDF files. Please see Section 3.3 for the full data file content.



4 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>

The datasets have been generated by University of Leicester and the points of contacts are the authors listed on the first page of this document.

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



12 References

- Boesch et al., 2011:** Boesch, H., D. Baker, B. Connor, D. Crisp, and C. Miller, Global characterization of CO₂ column retrievals from shortwave-infrared satellite observations of the Orbiting Carbon Observatory-2 mission, *Remote Sensing*, 3 (2), 270-304, 2011.
- Boesch et al., 2019:** Boesch, H., Anand, J., and Di Noia, A.: Algorithm Theoretical Basis Document (ATBD) – ANNEX A for products CO₂_GOS_OCFP, CH₄_GOS_OCFP & CH₄_GOS_OCPR (v7.2, 2009-2018), project C3S_312b_Lot2_DLR – Atmosphere, v3.1, 2019.
- Connor et al., 2008:** Connor, B. J., Boesch, H., Toon, G., Sen, B., Miller, C., and Crisp, D.: Orbiting Carbon Observatory: Inverse method and prospective error analysis, *J. Geophys. Res.*, 113, D05305, doi:10.1029/2006JD008336, 2008.
- Fischler and Bolles, 1981:** Fischler, M. A., and Bolles, R. C.: Random Sample Consensus: A paradigm for model fitting with applications to image analysis and automated cartography, *Comm. ACM*. 24, 381-395, doi: 10.1145/358669.358692, 1981
- Kataoka et al., 2019:** Kataoka, F., Knuteson, R. O., Kuze, A., Shiomi, K., Suto, H., Yoshida, J., Kondo, S., and Saitoh, N., Calibration, Level 1 processing, and radiometric validation for TANSO-FTS TIR on GOSAT, *IEEE Trans. Geosci. Remote Sens.*, 57, 3490-3500, doi: 10.1109/TGRS.2018.2885162, 2019.
- Kuze et al., 2009:** Kuze, A., Suto, H., Nakajima, M., and Hamazaki, T. (2009), Thermal and near infrared sensor for carbon observation Fourier-transform spectrometer on the Greenhouse Gases Observing Satellite for greenhouse gases monitoring, *Appl. Opt.*, 48, 6716–6733, 2009.
- Natraj et al., 2008:** Natraj, V., Boesch, H., Spurr, R. J. D., and Yung, Y. L.: Retrieval of XCO₂ from simulated Orbiting Carbon Observatory measurements using the fast linearized R-2OS radiative transfer model, *Journal of Geophysical Research D: Atmospheres*, 113(11), 2008.
- O'Dell, 2010:** O'Dell, C. W.: Acceleration of multiple-scattering, hyper-spectral radiative transfer calculations via low-streams interpolation, *Journal of Geophysical Research D: Atmospheres*, 115(10), 2010.
- Parker et al., 2011:** Parker, R., Boesch, H., Cogan, A., et al., Methane Observations from the Greenhouse gases Observing SATellite: Comparison to ground-based TCCON data and Model Calculations, *Geophys. Res. Lett.*, doi: 10.1029/2011GL047871, 2011.
- Parker et al., 2015:** Parker, R. J., Boesch, H., Byckling, K., Webb, A. J., Palmer, P. I., Feng, L., Bergamaschi, P., Chevallier, F., Notholt, J., Deutscher, N., Warneke, T., Hase, F., Sussmann, R., Kawakami, S., Kivi, R., Griffith, D. W. T., and Velazco, V.: Assessing 5 years of GOSAT Proxy XCH₄ data and associated uncertainties, *Atmos. Meas. Tech.*, 8, 4785- 4801, doi:10.5194/amt-8-4785-2015, 2015.
- Parker et al. 2020:** Parker, R. J., Webb, A., Boesch, H., Somkuti, P, Barrio Guillo, R., et al: A decade of GOSAT proxy satellite CH₄ observations, *Earth Syst. Sci. Data*, 12, 3383-3412, doi: 10.5194/essd-12-3383-2020
- Saitoh et al., 2009:** Saitoh, N., Imasu, R., Ota, Y., and Niwa, Y.: CO₂ retrieval algorithm for the thermal infrared spectra of the greenhouse gases observing satellite: Potential of retrieving CO₂



vertical profile from high-resolution FTS sensor, *Journal of Geophysical Research D: Atmospheres*, 114(17), 2009.

Somkuti et al., 2017: Somkuti, P., Boesch, H., Natraj, V., Kopparla, P., Application of a PCA - Based Fast Radiative Transfer Model to XCO₂ Retrievals in the Shortwave Infrared, *Journal of Geophysical Research: Atmospheres*, 122(19), doi: 10.1002/2017JD027013, 2017.

Spurr, 2008: Spurr, R.: LIDORT and VLIDORT: Linearized pseudo-spherical scalar and vector discrete ordinate radiative transfer models for use in remote sensing retrieval problems. In *Light Scattering Reviews 3* (pp. 229-275). Springer Berlin Heidelberg, 2008.

Spurr et al., 2011: Spurr, R., & Natraj, V.: A linearized two-stream radiative transfer code for fast approximation of multiple-scatter fields. *Journal of Quantitative Spectroscopy and Radiative Transfer*, 112(16), 2630-2637, 2011.

TRD GHG, 2017: Buchwitz, M., Aben, I., Anand, J., Armante, R., Boesch, H., Crevoisier, C., Detmers, R. G., Hasekamp, O. P., Reuter, M., Schneising-Weigel, O., Target Requirement Document, 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, 28-March-2017, pp. 52, 2017.

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.

Yokota et al., 2009: Yokota, T., Yoshida, Y., Eguchi, N., Ota, Y., Tanaka, T., Watanabe, H., and Maksyutov, S.: Global concentrations of CO₂ and CH₄ retrieved from GOSAT: First preliminary results, *Sola*, 5, 160-163, doi: 10.2151/sola.2009-041, 2009.

