



# **Product User Guide and Specification (PUGS) – ANNEX A for products CO2\_GOS\_OCFP, CH4\_GOS\_OCFP & CH4\_GOS\_OCPR**

## **C3S\_312a\_Lot6\_IUP-UB – Greenhouse Gases**

Issued by: Hartmut Boesch and Jasdeep Anand, University of Leicester,  
Leicester, UK

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## Contributors

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

M. Buchwitz

**UNIVERSITY OF LEICESTER, LEICESTER, UK  
(UoL)**

H. Boesch

J. Anand

P. Somkuti

R. Parker



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## History of modifications

| Version | Date            | Description of modification    | Chapters / Sections |
|---------|-----------------|--------------------------------|---------------------|
| 1.0     | 21-August-2017  | New document                   | All                 |
| 1.0b    | 11-October-2017 | Page header logo replaced      | Page header         |
| 1.3     | 20-October-2017 | Reference to main PUGS updated | Page 6              |
|         |                 |                                |                     |
|         |                 |                                |                     |



## Related documents

| Reference ID | Document  |
|--------------|---|
| D1           | Main PUGS:<br>Buchwitz, M., et al., Product User Guide and Specification (PUGS) – Main document, C3S project C3S_312a_Lot6_IUP-UB – Greenhouse Gases, 1.3, 2017.<br><i>(this document is an ANNEX to the Main PUGS)</i> |



## Acronyms

| Acronym   | Definition  |
|-----------|---|
| 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  |
| 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  |
| ppb       | Parts per billion   |
| ppm       | Parts per million   |
| PR        | (light path) PROxy retrieval method   |
| PQAR      | Product Quality Assessment Report   |
| SWIR      | Short Wave Infra Red  |
| TANSO     | Thermal And Near infrared Sensor for carbon Observation                       |
| TANSO-FTS | Fourier Transform Spectrometer on GOSAT                                       |
| TCCON     | Total Carbon Column Observing Network   |



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|     |   |
|-----|---|
| TIR | Thermal Infra Red                       |
| TR  | Target Requirements                     |
| TRD | Target Requirements Document            |
| UoL | University of Leicester, United Kingdom |





## General definitions

Table 1 lists some general definitions relevant for this document.

Table 1: General definitions.

| Item             | Definition  |
|------------------|---|
| XCO <sub>2</sub> | Column-averaged dry-air mixing ratios (mole fractions) of CO <sub>2</sub>   |
| XCH <sub>4</sub> | Column-averaged dry-air mixing ratios (mole fractions) of CH <sub>4</sub>   |
| L1               | Level 1 satellite data product: geolocated radiance (spectra)   |
| L2               | Level 2 satellite-derived data product: Here: CO <sub>2</sub> and CH <sub>4</sub> information for each ground-pixel                     |
| L3               | Level 3 satellite-derived data product: Here: Gridded CO <sub>2</sub> and CH <sub>4</sub> information, e.g., 5 deg times 5 deg, monthly |
| L4               | Level 4 satellite-derived data product: Here: Surface fluxes (emission and/or uptake) of CO <sub>2</sub> and CH <sub>4</sub>            |



## Scope of document

This document is a Product User Guide and Specification (PUGS) for the Copernicus Climate Change Service (C3S, <https://climate.copernicus.eu/>) component as covered by project C3S\_312a\_Lot6 led by University of Bremen, Germany.

Within project C3S\_312a\_Lot6 satellite-derived atmospheric carbon dioxide (CO<sub>2</sub>) and methane (CH<sub>4</sub>) 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 C3S\_312a\_Lot 6 satellite-derived data products are:

- Column-averaged dry-air mixing ratios (mole fractions) of CO<sub>2</sub> and CH<sub>4</sub>, denoted XCO<sub>2</sub> (in parts per million, ppm) and XCH<sub>4</sub> (in parts per billion, ppb), respectively.
- Mid/upper tropospheric mixing ratios of CO<sub>2</sub> (in ppm) and CH<sub>4</sub> (in ppb).

This document describes the C3S products CO2\_GOS\_OCFP (v 7.1), CH4\_GOS\_OCFP (v 7.1) and CH4\_GOS\_OCPR (v 7.0).

These products are XCO<sub>2</sub> and XCH<sub>4</sub> 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 CO<sub>2</sub> and CH<sub>4</sub> data products developed by the University of Leicester (UoL). These products provide the column-averaged dry-air mixing ratios (mole fractions) of CO<sub>2</sub> (XCO<sub>2</sub>) and (XCH<sub>4</sub>), 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 (2009-2016), and is published as daily netCDF files available from the C3S website: <https://climate.copernicus.eu/>.

This aim of this document is to clearly describe to users the quality flags and metadata, data format, product grid and geographical projection, known limitations, 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*, through comparisons with highly accurate ground-based measurements provided by the Total Carbon Column Observing Network (TCCON). Through these comparisons, we are confident 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 thought to offer information on regional surface fluxes of CO<sub>2</sub> and CH<sub>4</sub>.



## 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 CO<sub>2</sub> and CH<sub>4</sub> from its SWIR bands, *Yoshida et al., 2013*. It is equipped with two instruments; the Thermal And Near infra-red Sensor for carbon Observations - Fourier Transform Spectrometer (TANSO-FTS), and a dedicated Cloud and Aerosol Imager (TANSO-CAI).

TANSO-FTS measures in four spectral bands with a high spectral resolution of 0.3 cm<sup>-1</sup>, three of which operate in the SWIR at around 0.76, 1.6 and 2.0 μm providing sensitivity to the near-surface absorbers with the fourth channel operating in the thermal infrared between 5.5 and 14.3 μm providing mid-tropospheric sensitivity, *Saitoh et al., 2009*.

The measurement strategy of TANSO-FTS is optimised for the characterisation of continental-scale sources and sinks, with the aim of achieving a 0.3—1% relative accuracy for 3-month averages of CO<sub>2</sub> at a 100-1000 km spatial resolution, *Kuze et al., 2009*. The aim for CO<sub>2</sub> is to achieve an accuracy of better than 2% on the same spatial and temporal scales. In order to achieve this, TANSO-FTS utilises a pointing mirror to perform off-nadir measurements at the same location on each 3-day repeat cycle. The pointing mirror allows TANSO-FTS to observe up to ±35° across track and ±20° along-track. These measurements nominally consist of 5 across track points spaced ~100km apart (although measurements are possible with 1, 3, 5, 7 or 9 across track points) with a ground footprint diameter of approximately 10.5 km and a 4 second exposure duration. Whilst the majority of data is limited to measurements over land where surface reflectance is high, TANSO-FTS also observes in sun-glint mode over the ocean within ±20° of the subsolar latitude.

### 1.2 The University of Leicester Products

The UoL have retrieved several datasets from GOSAT TANSO-FTS NIR and SWIR spectra, which are discussed in this section:

XCO<sub>2</sub>:

- CO2\_GOS\_OCFP (v 7.1)

XCH<sub>4</sub>:

- CH4\_GOS\_OCFP (v 7.1)
- CH4\_GOS\_OCPR (v 7.0)



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 addition, we use the low-streams interpolation functionality of the code, *O'Dell, 2010*, to accelerate the radiative transfer component of the retrieval algorithm.

In addition to the Full-Physics retrieval products, we also offer a separate product for CH<sub>4</sub>, which is retrieved using the Full-Physics algorithm modified by the “proxy” technique (OCPR) as discussed in, *Parker et al., 2011* and, *Parker et al., 2015*. CO<sub>2</sub> is known to vary in the atmosphere much less than CH<sub>4</sub> and as the CO<sub>2</sub> absorption band is spectrally close to that of CH<sub>4</sub> we can use the CO<sub>2</sub> as a proxy for the light path to minimize common spectral artefacts due to aerosol scattering and instrumental effect. CH<sub>4</sub> and CO<sub>2</sub> 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<sub>4</sub>, it is necessary to multiply the retrieved XCH<sub>4</sub>/XCO<sub>2</sub> ratio by a model XCO<sub>2</sub>. We obtain the CO<sub>2</sub> VMRs from the median of a model CO<sub>2</sub> ensemble that comprises of GEOS-Chem (University of Edinburgh), LMDZ/MACC-II and NOAA CarbonTracker, convolved with scene-dependent instrument averaging kernels obtained from the GOSAT 1.6 μm CO<sub>2</sub> retrieval.

Figures 1-3 show the global seasonal variation of XCO<sub>2</sub> and XCH<sub>4</sub> over all three data products between April 2009 and December 2016.





Figure 1: Global seasonal maps of UoL GOSAT XCO<sub>2</sub> (CO<sub>2</sub>\_GOS\_OCFP) retrieved between April 2009 and December 2016.

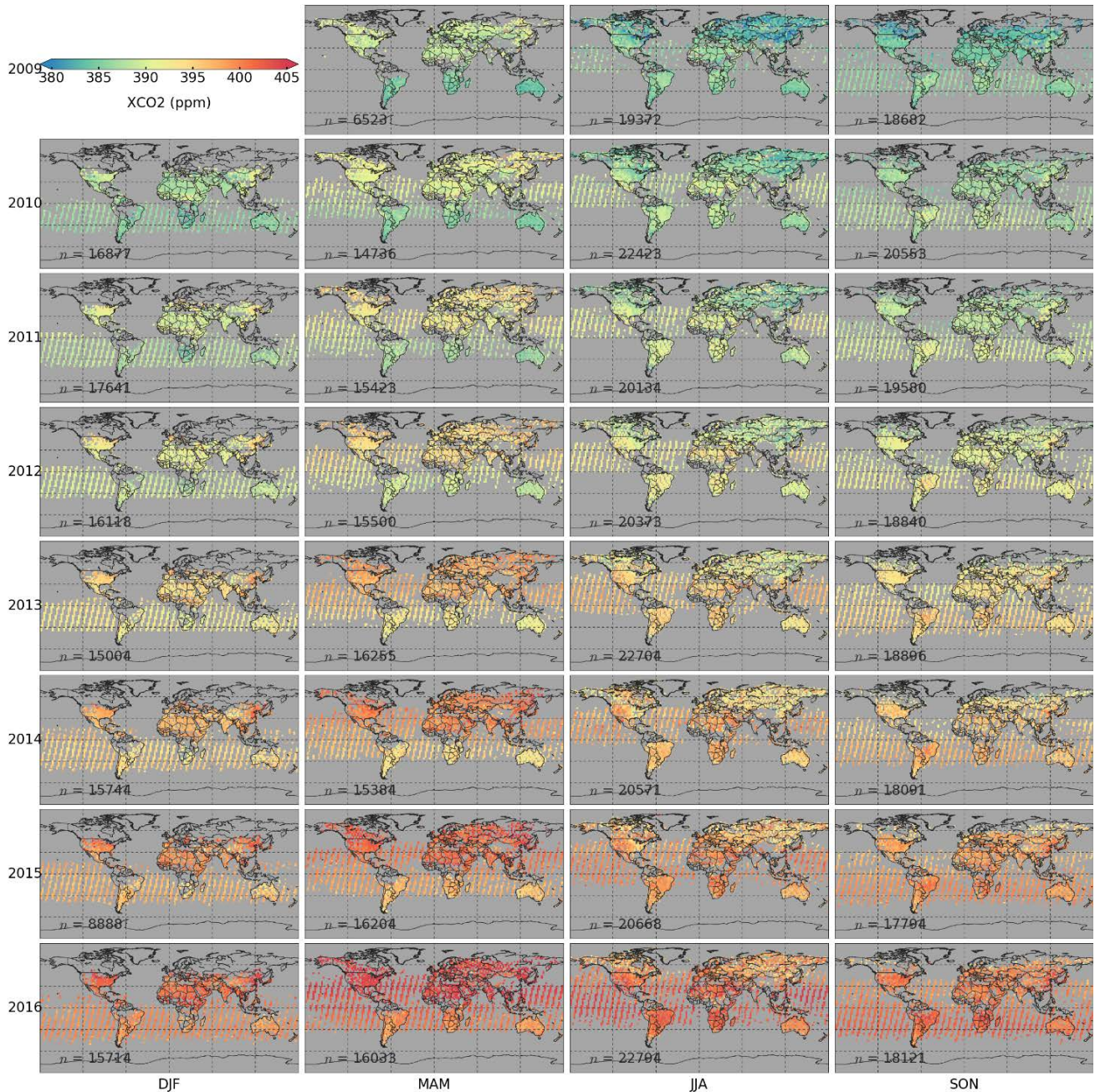




Figure 2: Global seasonal maps of UoL GOSAT XCH<sub>4</sub> (CH<sub>4</sub>\_GOS\_OCFP) retrieved between April 2009 and December 2016.

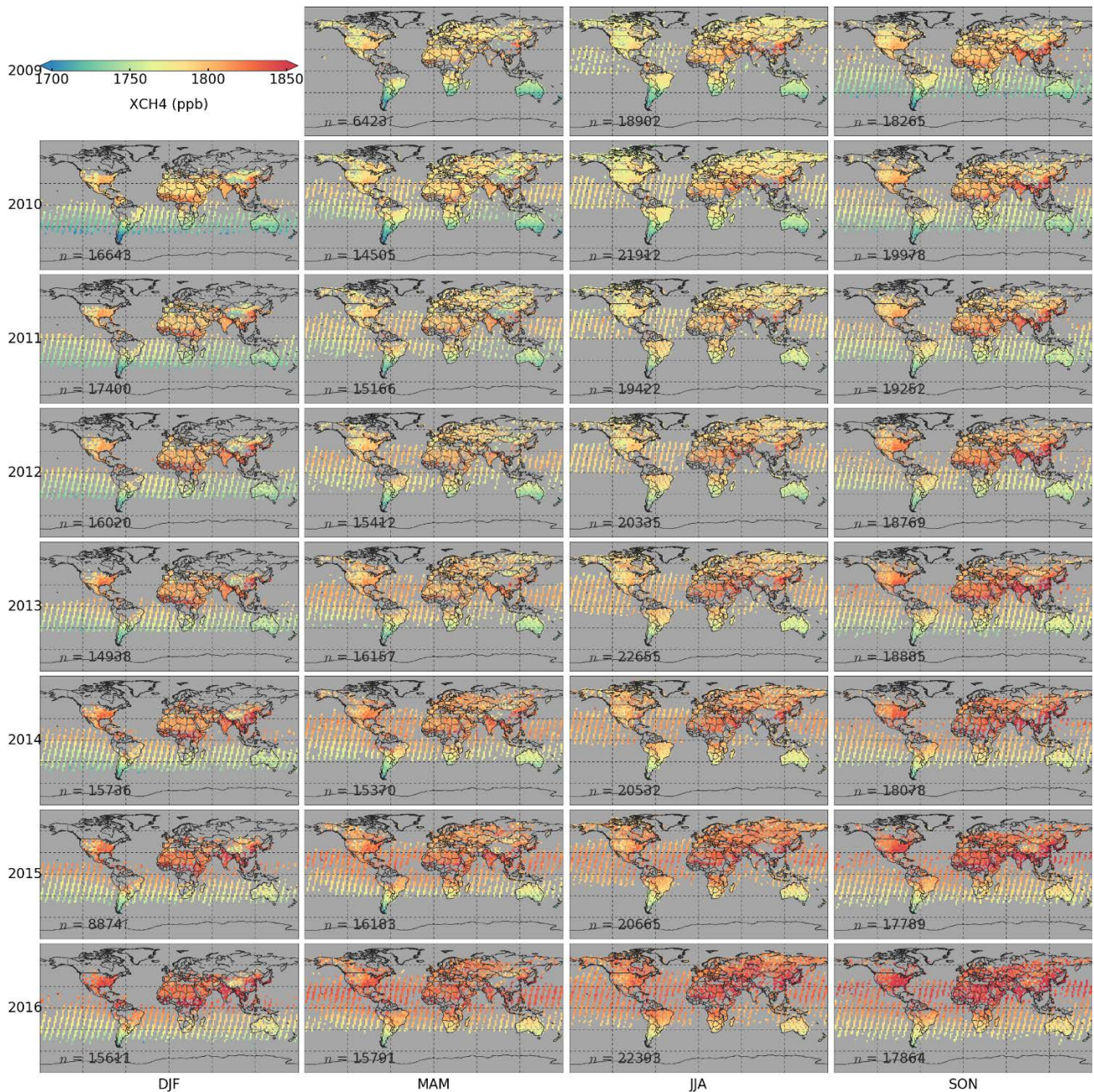
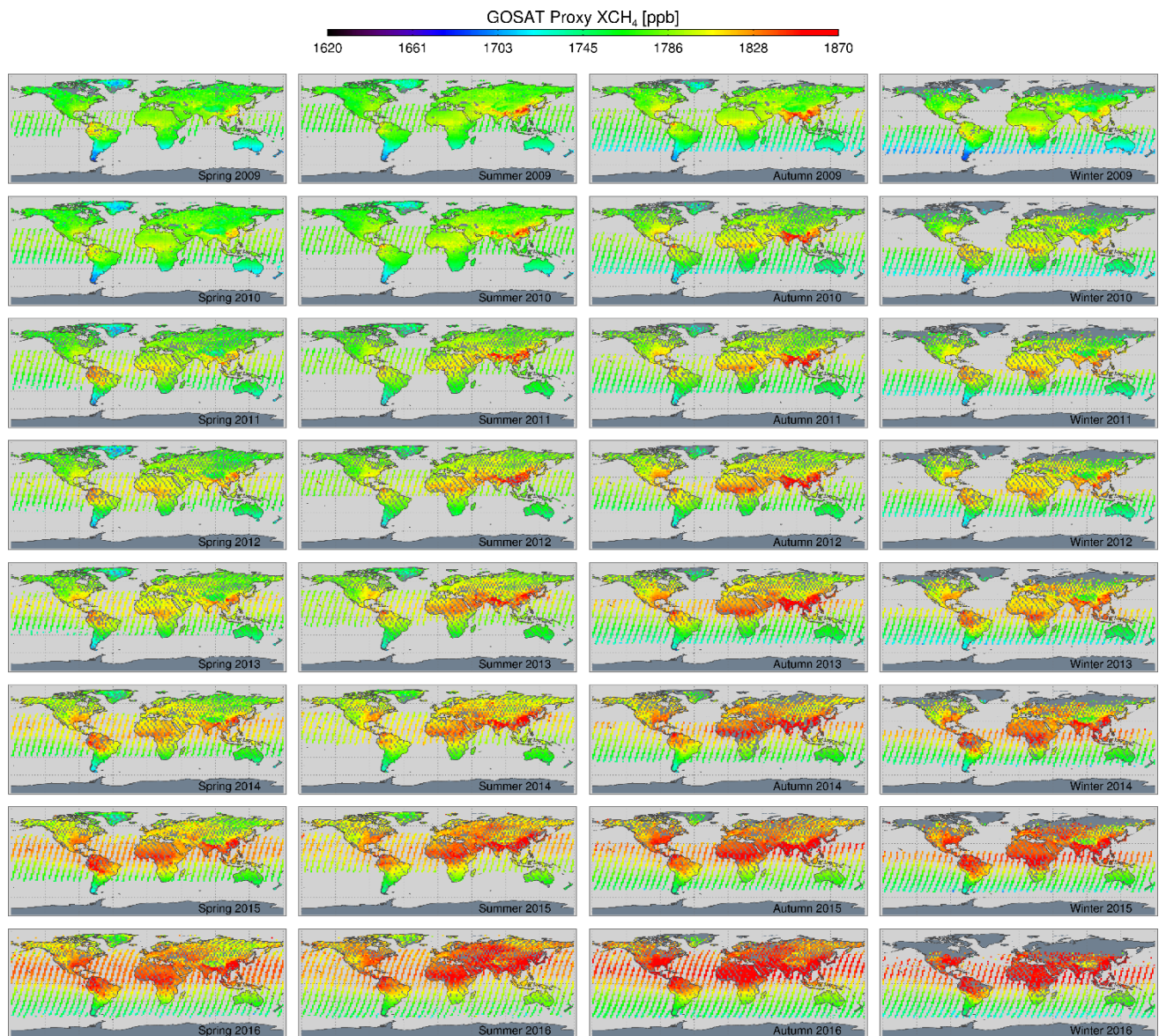




Figure 3: Global seasonal maps of UoL GOSAT XCH<sub>4</sub> (CH<sub>4</sub>\_GOS\_OCPR) retrieved between April 2009 and December 2016.



### 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 was 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).





### 1.3.1.1 Pre-retrieval screening

Before a retrieval is performed the GOSAT soundings are subjected to several tests for measurements noise and other issues. For CO<sub>2</sub>\_GOS\_OCFP and CH<sub>4</sub>\_GOS\_OCFP, only soundings that pass the criteria shown in Table 2 are used in the retrieval. For the CH<sub>4</sub>\_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 CO<sub>2</sub>\_GOS\_OCFP and CH<sub>4</sub>\_GOS\_OCFP product.

| Parameter   | Filtering criteria        |
|---|---------------------------|
| SNR (all bands)   | $\geq 20$                 |
| SZA   | $\leq 75^\circ$           |
| Latitude  | $\geq 60^\circ \text{ S}$ |
| $\Delta$ (Surface pressure): difference between retrieved and a priori value (cloud screen) | $\leq 30 \text{ hPa}$     |
| Weak/strong CO <sub>2</sub> column ratio  | $\geq 0.98, \leq 1.05$    |

### 1.3.1.2 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 CO<sub>2</sub>\_GOS\_OCFP are shown in Table 3. For CH<sub>4</sub>\_GOS\_OCFP only soundings which had previously passed the CO<sub>2</sub>\_GOS\_OCFP filtering were considered useful. The CH<sub>4</sub> retrievals from these soundings were then subsequently tested for divergence and the number of iterations using the same criteria shown in Table 3 before being flagged as good data.



Table 3: The post-retrieval filtering criteria used in the CO<sub>2</sub>\_GOS\_OCFP product. For CH<sub>4</sub>\_GOS\_OCFP the same soundings that passed the CO<sub>2</sub>\_GOS\_OCFP filtering were used, after being filtered using the same criteria for divergence and number of iterations.

| Parameter   | Filtering criteria         |   |
|---|----------------------------|---|
|   | Land                       | Glint   |
| SNR (all bands)   | $\geq 45$                  | $\geq 45$   |
| $n$ retrieval iterations  | $\leq 7$                   | $\leq 7$  |
| SZA   | $\leq 65^\circ$            | NA  |
| $n$ diverging retrieval steps   | $\leq 2$                   | $\leq 2$  |
| $\chi^2$ (Band 1)   | $\geq 0.5, \leq 1.55$      | $\geq 0.99, \leq 1.45$                              |
| $\chi^2$ (Band 2)   | $\geq 0.6, \leq 2.0$       | $\geq 0.8, \leq 1.70$                               |
| $\chi^2$ (Band 3)   | $\geq 0.5, \leq 1.55$      | $\geq 0.65, \leq 1.25$                              |
| Weak/strong CO <sub>2</sub> column ratio  | $\geq 0.99, \leq 1.01$     | $\geq 0.99, \leq 1.01$                              |
| XCO <sub>2</sub> a posteriori error   | $\leq 2.5$ ppm             | $\leq 1.15$ ppm                                     |
| Total AOD (cirrus + small + large aerosols)   | $\leq 0.5$                 | $\leq 0.17$   |
| AOD (small aerosol)   | $\leq 0.3$                 | $\leq 0.3$  |
| AOD (large aerosol)   | $\leq 0.1$                 | $\leq 0.08$   |
| $\Delta$ AOD (large aerosol): difference between retrieved and a priori value               | $\geq -1.8$                | $\geq -1.25$  |
| $\Delta$ AOD (cirrus): difference between retrieved and a priori value                      | $\geq -6.25$               | $\geq -7.0$   |
| $\sigma$ retrieved surface pressure   | $\leq 20$ hPa              | NA  |
| $\Delta$ (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  | $\leq 2.75$                | $\geq 0.98, \leq 1.2$                               |
| Albedo ratio between band 1 and band 3  | NA                         | $\geq 1.09, \leq 1.2$                               |
| Retrieved CO <sub>2</sub> profile   | NA                         | $\geq 0.9, \leq 1.01$                               |



|   |  |  |
|---|--|--|
| gradient between the surface and retrieval level 15 |  |  |
|---|--|--|

The post-retrieval filter criteria used in the CH4\_GOS\_OCPR product is the same for both land and glint soundings, and is shown in Table 4.

Table 4: The post-retrieval filtering criteria used in the CO2\_GOS\_OCPR product.

| Parameter                             | Filtering criteria   |
|---------------------------------------|----------------------|
| $\chi^2$ (XCH <sub>4</sub> retrieval) | $\geq 0.4, \leq 1.9$ |
| $\chi^2$ (XCO <sub>2</sub> retrieval) | $\geq 0.4, \leq 1.9$ |
| XCH <sub>4</sub> a posteriori error   | $\leq 20$ ppb        |
| XCO <sub>2</sub> a posteriori error   | $\leq 3$ ppm         |
| Retrieved XCH <sub>4</sub>            | $\geq 1650$ ppb      |
| Retrieved XCO <sub>2</sub>            | $\geq 350$ ppm       |

### 1.3.2 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 XCH<sub>4</sub> and XCO<sub>2</sub> 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 ( $x$ ) multiplied by a unique coefficient ( $m$ ) along with a single offset ( $c$ ), such that:

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

The correction is then subtracted from the original XCO<sub>2</sub> or XCH<sub>4</sub> to give the final value:

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

The regression analysis makes use of the RANSAC method 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 5-8 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 5: The parameters and coefficient values used in the bias correction for the CO<sub>2</sub>\_GOS\_OCFP product (land soundings only). An offset of: -16.17 ppm is also applied.

| Parameter   | Coefficient |
|---|-------------|
| Retrieved CO <sub>2</sub> profile gradient between the surface and retrieval level 15 | 17.42       |
| Retrieved zero-level offset in band 1   | 164.46      |

Table 6: The parameters and coefficient values used in the bias correction for the CO<sub>2</sub>\_GOS\_OCFP product (glint soundings only). An offset of: 5.57 ppm is also applied.

| Parameter   | Coefficient            |
|---|------------------------|
| Albedo slope (Band 3)   | $-1.45 \times 10^3$    |
| Retrieved CO <sub>2</sub> profile gradient between the surface and retrieval level 15 | -5.35                  |
| Total AOD (cirrus + small + large aerosols)   | $-1.77 \times 10^{-2}$ |
| Albedo slope (Band 1)   | 2.81                   |

Table 7: The parameters and coefficient values used in the bias correction for the CH<sub>4</sub>\_GOS\_OCFP product (land soundings only). An offset of: -51.80 ppb is also applied.

| Parameter   | Coefficient |
|---|-------------|
| Albedo ratio between band 1 and band 3  | 3.84        |
| Total AOD (cirrus + small + large aerosols)   | -61.75      |
| Retrieved CO <sub>2</sub> profile gradient between the surface and retrieval level 15 | 42.21       |

Table 8: The parameters and coefficient values used in the bias correction for the CH<sub>4</sub>\_GOS\_OCFP product (glint soundings only). An offset of: 112.30 ppb is also applied.

| Parameter                              | Coefficient         |
|--|---------------------|
| AOD (small aerosol)                    | $-1.21 \times 10^2$ |
| Albedo slope (Band 2)                  | $-5.80 \times 10^5$ |
| Albedo ratio between band 1 and band 3 | $-8.60 \times 10^1$ |

For CH<sub>4</sub>\_GOS\_OCPR a simple global bias correction of -7.36 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 9 shows the random and systematic errors stated in the TRD.



Table 9: XCO<sub>2</sub> and XCH<sub>4</sub> 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 <sub>2</sub> and XCH <sub>4</sub> |           |                            |   |                         |                                  |
|--|-----------|----------------------------|---|-------------------------|----------------------------------|
| Parameter  | Req. type | Random error (“Precision”) |   | Systematic error        | Stability                        |
|  |           | Single obs.                | 1000 <sup>2</sup> km <sup>2</sup> monthly |                         |                                  |
| XCO <sub>2</sub>   | 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 <sub>4</sub>   | 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 10 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 XCO<sub>2</sub> and XCH<sub>4</sub> stated in Table 9.

Table 10: The results of direct comparisons between the UoL products and TCCON for GOSAT soundings between April 2009 and December 2016.

| Dataset                       | Number of measurements | Pearson coefficient (r) | Mean bias | Standard deviation |
|-------------------------------|------------------------|-------------------------|-----------|--------------------|
| CO <sub>2</sub> (land)        | 15796                  | 0.94                    | 0.02 ppm  | 1.87 ppm           |
| CO <sub>2</sub> (glint)       | 671                    | 0.95                    | -0.05 ppm | 1.23 ppm           |
| CH <sub>4</sub> (OCFP, land)  | 15634                  | 0.88                    | -0.03 ppb | 14.38 ppb          |
| CH <sub>4</sub> (OCFP, glint) | 822                    | 0.91                    | 0.80 ppb  | 10.52 ppb          |
| CH <sub>4</sub> (OCP, all)    | 52052                  | 0.90                    | 0.06 ppb  | 13.43 ppb          |



### 3. Data usage information

For all data products, the **xco2\_quality\_flag** or **xch4\_quality\_flag** variable must be applied to the data before use; a value of 0 indicates that the data has passed our quality control. 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<sub>4</sub>/XCO<sub>2</sub> ratio. Users interested in the raw XCH<sub>4</sub> and XCO<sub>2</sub> retrieved from the 1.6  $\mu\text{m}$  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.

#### 3.1 Tools for reading the data

The datasets are stored in netCDF format, which can be read with standard tools in common programming languages.

#### 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<sub>2</sub> and XCH<sub>4</sub> 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 1.55 so that it is a more realistic value, while the xch4\_uncertainty reported in the CH4\_GOS\_OCFP product has been multiplied by a factor of 1.70. 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<sub>2</sub> column can be found in Section 1.2. If you wish to renormalize the XCH<sub>4</sub>/XCO<sub>2</sub> ratio with your own model XCO<sub>2</sub> 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. A dimension of  $n$  refers to the number of retrievals per file, whilst a dimension of  $m$  refers to the number of levels retrieved for each sounding (typically 20).

Table 11: 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 <sub>2</sub> ) in ppm.   |
| xco2_no_bias_correction | float  | n          | 1e-6                              | Retrieved column-averaged dry-air mole fraction of atmospheric carbon dioxide (XCO <sub>2</sub> ) in ppm. No bias correction is applied                   |
| xco2_uncertainty        | float  | n          | 1e-6                              | Statistical uncertainty of XCO <sub>2</sub> in ppm (1 $\sigma$ )  |
| xco2_averaging_kernel   | float  | n, m       |                                   | XCO <sub>2</sub> averaging kernel (a profile = vector for each single observation). Quantifies the altitude sensitivity of the XCO <sub>2</sub> retrieval |
| co2_profile_apriori     | float  | n, m       | 1e-6                              | A-priori mole fraction profile of atmospheric CO <sub>2</sub> 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 <sub>2</sub> 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 12: Variables present in the CH<sub>4</sub>\_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 <sub>4</sub> ) in ppb.  |
| xch4_no_bias_correction          | float | n     | 1e-9   | Retrieved column-averaged dry-air mole fraction of atmospheric methane (XCH <sub>4</sub> ) in ppb. No bias correction is applied                          |
| xch4_uncertainty                 | float | n     | 1e-9   | Statistical uncertainty of XCH <sub>4</sub> in ppb (1σ)   |
| xch4_averaging_kernel            | float | n, m  |        | XCH <sub>4</sub> averaging kernel (a profile = vector for each single observation). Quantifies the altitude sensitivity of the XCH <sub>4</sub> retrieval |
| co2_profile_apriori              | float | n, m  | 1e-6   | A-priori mole fraction profile of atmospheric CO <sub>2</sub> in ppm  |
| ch4_profile_apriori              | float | n, m  | 1e-9   | A-priori mole fraction profile of atmospheric CH <sub>4</sub> 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 <sub>2</sub> 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 CH<sub>4</sub>\_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 <sub>4</sub> ) in ppb.  |
| xch4_uncertainty      | float  | n          | 1e-9                              | Statistical uncertainty of XCH <sub>4</sub> in ppb (1σ)   |
| xch4_averaging_kernel | float  | n, m       |                                   | XCH <sub>4</sub> averaging kernel (a profile = vector for each single observation). Quantifies the altitude sensitivity of the XCH <sub>4</sub> retrieval |
| co2_profile_apriori   | float  | n, m       | 1e-6                              | A-priori mole fraction profile of atmospheric CO <sub>2</sub> in ppm  |
| ch4_profile_apriori   | float  | n, m       | 1e-9                              | A-priori mole fraction profile of atmospheric CH <sub>4</sub> in ppb  |
| raw_xco2              | float  | n          | ppm                               | Retrieved 1.6μm XCO <sub>2</sub>  |
| raw_xch4              | float  | n          | ppb                               | Retrieved 1.6μm XCH <sub>4</sub>  |
| raw_xco2_error        | float  | n          | ppm                               | Retrieved 1.6μm XCO <sub>2</sub> error  |
| raw_xch4_error        | float  | n          | ppb                               | Retrieved 1.6μm XCH <sub>4</sub> error  |
| model_xco2            | float  | n          | ppm                               | Model XCO <sub>2</sub> component of the final proxy data product  |



|                                  |       |       |        |  |
|----------------------------------|-------|-------|--------|--|
| model_xco2_range                 | float | n     | ppm    | Maximum difference (in ppm) between model XCO <sub>2</sub> 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 <sub>2</sub> 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)  |



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ECMWF - Shinfield Park, Reading RG2 9AX, UK

Contact: [info@copernicus-climate.eu](mailto:info@copernicus-climate.eu)