ESA Climate Change Initiative “Plus” (CCI+)

Product User Guide (PUG)
XCH₄ via RemoTeC from GOSAT2
(CH₄_GO2_SRPR)
for the Essential Climate Variable (ECV)
Greenhouse Gases (GHG)

Version 1.1 (PUGv1.1)

for the RemoTeC XCH₄ GOSAT2 Data Product
CH₄_GO2_SRPR (v1.0.0)

for the Essential Climate Variable (ECV)
Greenhouse Gases (GHG)

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<table>
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<th>Version Nr.</th>
<th>Date</th>
<th>Status</th>
<th>Reason for change</th>
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<tr>
<td></td>
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<td>- Update purpose of document</td>
</tr>
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<td>- Remove typos</td>
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</tbody>
</table>
Table of Contents

1. Purpose of document ................................................................. 4

2. Greenhouse gases Observing SATellite-2 (GOSAT-2) .................. 5

3. RemoTeC retrieval algorithm ....................................................... 6

4. XCH₄ data product (RemoTeC-PROXY, Feb-October 2019) .......... 7
   4.1 Global maps ........................................................................... 7
   4.2 Validation with TCCON .......................................................... 9
   4.3 Bias correction .................................................................... 12

5. Description of data format .......................................................... 13
   5.1 Product Content and Format .................................................. 13
   5.2 Quality Flags and Metadata .................................................... 17
   5.3 Recommended data usage ...................................................... 18
   5.4 Tools for Reading the Data .................................................... 18

6. References .................................................................................. 19
1. Purpose of document

This document describes the Product User Guide (PUG) of the CH4_GO2_SRFP product which is a deliverable for the ESA GHG-CCI+ project led by University of Bremen, Germany.

Within the project satellite-derived atmospheric carbon dioxide (CO\textsubscript{2}) and methane (CH\textsubscript{4}) Essential Climate Variable (ECV) data products are generated and delivered to ESA for inclusion into the ESA-GHG-CCI+ database from which users can access these data products and the corresponding documentation.

The satellite-derived data products are:

- Column-averaged dry-air mixing ratios (mole fractions) of CO\textsubscript{2} and CH\textsubscript{4}, denoted XCO\textsubscript{2} (in parts per million, ppm) and XCH\textsubscript{4} (in parts per billion, ppb), respectively.

This document will be focused on the XCH\textsubscript{4} Level-2 product retrieved using the GOSAT-2 Proxy algorithm developed by SRON Netherlands Institute for Space Research, The Netherlands.
2. Greenhouse gases Observing SATellite-2 (GOSAT-2)

The Japanese Greenhouse gases Observing SATellite-2 (GOSAT2) was launched on 29th October 2018 and started operational observations from February 2019. GOSAT2 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) as well as a dedicated Cloud and Aerosol Imager-2 (TANSO-CAI-2).

The TANSO-FTS2 instrument (Nakajima et al., 2017) has five spectral bands with a high spectral resolution 0.2 cm$^{-1}$. Three operate in the SWIR at 0.75-0.77, 1.56-1.69 and at the extended 1.92-2.33 μm range, providing sensitivity to the near-surface absorbers. The fourth and fifth channels operating in the thermal infrared between 5.5-8.4 and 8.4-14.3 μm providing mid-tropospheric sensitivity.

The measurement strategy of TANSO-FTS2 is optimized for the characterization of continental-scale sources and sinks. TANSO-FTS2 utilizes a pointing mirror to perform off-nadir measurements at the same location on each 6-day repeat cycle. The pointing mirror allows TANSO-FTS2 to observe up to ±35° across track and ±40° along-track. These measurements nominally consist of 5 across track points spaced ~160 km apart with a ground footprint diameter of approximately 9.7 km and a 4 second exposure duration. The satellite has an intelligent pointing monitor camera which makes it possible to adjust the line of sight of the FTS to steer away from cloud contaminated areas. Whilst the majority of data is limited to measurements over land where the surface reflectance is high, TANSO-FTS2 also observes in sunglint mode over the ocean.
3. RemoTeC retrieval algorithm

The CH4_GO2_SRPR product is retrieved from GOSAT-2 TANSO-FTS SWIR spectra using the RemoTeC algorithm that has been jointly developed at SRON and KIT. The algorithm retrieves simultaneously XCH$_4$ and XCO$_2$. 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 XCO$_2$ and XCH$_4$ 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 XCH$_4$ column cannot be used directly, as effects of aerosol scattering modify the light path. To correct for this, in the PROXY approach, the retrieved XCH$_4$ column is divided by the retrieved XCO$_2$ column at the 1.61 µm band and then multiplied by a XCO$_2$ total column obtained from the Copernicus Atmosphere Monitoring Service (CAMS) v18r2 product (Chevallier et al., 2019).

The retrieved XCH$_4$ has been validated with ground based TCCON measurements. To further improve accuracy a bias correction has been developed based on TCCON comparisons. We use the GGG2014 release of the TCCON data (Wunch et al., 2015). More details on the technical aspects of the retrievals can be found in the ATBD GO2-SRPR document (ATBDv1.1, 2020).
4. XCH₄ data product (RemoTeC-PROXY, Feb-October 2019)

In this section, we show examples of the new GOSAT-2 XCH₄ PROXY data product by showing averaged maps (Sect. 4.1) and by giving a summary of the validation results relative to TCCON (Sect. 4.2).

4.1 Global maps

Figure 1 and Figure 2 show global mean maps of the RemoTeC GOSAT-2 XCH₄ PROXY data product. Figure 1 shows the bias-corrected XCH₄ data and Figure 2 the scaled random error, which is described in detail in (E3UBv1.1, 2020). As can be seen, the spatial coverage is limited by cloud-cover (the observations correspond to cloud free scenes), sun illumination conditions, etc.

![Global XCH₄ [ppb] map](image)

**Figure 1:** Global XCH₄ [ppb] for the February-2019 - October 2019 period for the CH4_GO2_SRPR product on a 2 by 2 degree resolution.
Figure 2: As Figure 1 but for the corresponding uncertainty.
4.2 Validation with TCCON

This section summarizes the main validation results presented in the RemoTeC GOSAT-2 ESA GHG CCI+ End-to-End ECV Uncertainty Budget Version 1.1 (E3UBv1.1, 2021) document.

We used ground based TCCON GGG2014 (Wunch et al., 2015) data obtained from http://tccon.orl.gov as reference data set. We co-located GOSAT-2 and TCCON measurements with a maximum time difference of 2h, a maximum distance of 2.5 degrees in both longitudinal and latitudinal directions. An altitude correction is applied to account for elevation differences.

In cases with multiple TCCON measurements of the same site co-locating with a GOSAT-2 sounding, we averaged the TCCON measurements. In total, we found about 2642 co-locations with TCCON during the nine-month validation period Feb-Oct 2019. As not all TCCON sites updated their datasets it was only possible to use 9 sites which limits the number of co-locations.

Figure 3 shows the co-locations of 9 sites with non-glint observations. Statistics per site statistics are shown in Figure 4. Detailed bias and scatter, i.e., single sounding precision measured by the standard deviation of the difference to TCCON after removing systematic effect are described in E3UBv1.1 (2021).

The standard deviation of the site biases (spatial accuracy) is 4.2 ppb. TCCON observes these gases with a precision on mole fractions of ~0.15% and ~0.2% for CO₂ and CH₄ respectively (Toon et al., 2009). The single measurement precision of GOSAT-2 compared to TCCON amounts to 15.3 ppb.

The validation results can be summarized as follows:

- Single measurement precision ("precision", 1-sigma): 15.3 ppb
- Mean bias (all observations, global offset): 0.10 ppb
- Spatial accuracy (standard deviation site biases): 4.2 ppb
Figure 3 Validation of non-glint single soundings of PROXY-CH₄ with co-located TCCON measurements at all TCCON sites for the period Feb-Oct 2019. Numbers in the figures: $\mu$ = bias, i.e., average of the difference; $\sigma$ = single measurement precision, i.e., standard deviation of the difference; N = number of co-locations.
**Figure 4:** Validation statistics bias (top) and scatter (bottom) per TCCON site for RemoTeC PROXY CH₄ (bias corrected). The summarizing values (“overall”) represent the standard deviation of the site biases and the average scatter relative to TCCON.
4.3 Bias correction

From comparison with TCCON it was found that the error in XCH$_4$ correlates with the retrieved albedo $\alpha$ at 1.6 um in band 2. Based on this correlation the following bias correction has been developed for XCH$_4$:

$$ XCH_4_{\text{corr}} = XCH_4 \ast (a + b \ast \alpha) $$

with $a = 0.9904$, $b = 0.0144$.

The bias correction parameters are obtained from fits to the GOSAT-2-TCCON differences.

For sunglint observations there were not enough co-located TCCON observations, therefor the parameter was obtained from comparison to GOSAT-1 data:

$$ XCH_4_{\text{corr}} = XCH_4 \ast a $$

with $a = 0.99445$. 
5. Description of data format

5.1 Product Content and Format

The RemoteC XCH4 data product is stored per day in a single NetCDF file. Retrieval results are provided for the individual GOSAT-2 spatial footprints. 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, quality of the fit.

Table 1: Common dimensions for the CH4_GO2_SRPR product

<table>
<thead>
<tr>
<th>Dimension</th>
<th>Type</th>
<th>Unlimited</th>
<th>Units</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>sounding_dim</td>
<td>int</td>
<td>no</td>
<td></td>
<td>Number of sounding</td>
</tr>
<tr>
<td>polarization_dim</td>
<td>int</td>
<td>no</td>
<td></td>
<td>Number of polarization = 2</td>
</tr>
<tr>
<td>level_dim</td>
<td>int</td>
<td>no</td>
<td></td>
<td>Number of level = 5</td>
</tr>
<tr>
<td>layer_dim</td>
<td>int</td>
<td>no</td>
<td></td>
<td>Number of layer = 4</td>
</tr>
<tr>
<td>window_dim</td>
<td>int</td>
<td>no</td>
<td></td>
<td>Number of retrieval window = 4</td>
</tr>
<tr>
<td>char_l1bname</td>
<td>int</td>
<td>no</td>
<td></td>
<td>Number of character of L1B name = 44</td>
</tr>
</tbody>
</table>

Table 2: Common variables for the CH4_GO2_SRPR product

<table>
<thead>
<tr>
<th>Variable</th>
<th>Type</th>
<th>Dim.</th>
<th>Units</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>solar_zenith_angle</td>
<td>float</td>
<td>sounding_dim</td>
<td>degrees</td>
<td>Angle between line of sight to the sun and local vertical</td>
</tr>
</tbody>
</table>
### Table 3: Product specific (additional) variables for the CH4_GO2_SRPR product

<table>
<thead>
<tr>
<th>Name</th>
<th>Type</th>
<th>Dim.</th>
<th>Units</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>flag_landtype</td>
<td>int</td>
<td>sounding_dim</td>
<td></td>
<td>0 = land, 1 = ocean</td>
</tr>
<tr>
<td>flag_sunglint</td>
<td>int</td>
<td>sounding_dim</td>
<td></td>
<td>0 = no sunglint, 1 = sunglint</td>
</tr>
<tr>
<td>gain</td>
<td>int</td>
<td>sounding_dim</td>
<td></td>
<td>gain setting of sensor</td>
</tr>
<tr>
<td>exposure_id</td>
<td>int</td>
<td>sounding_dim</td>
<td></td>
<td>Exposure identification number of the sounding</td>
</tr>
</tbody>
</table>

**sensor_zenith_angle**  
float  
sounding_dim  
degrees  
Angle between the line of sight to the sensor and the local vertical

**time**  
float  
sounding_dim  
seconds  
Seconds since 1970-01-01 00:00:00

**longitude**  
float  
sounding_dim  
degrees _east  
Center longitude

**latitude**  
float  
sounding_dim  
degrees _north  
Center latitude

**pressure_levels**  
float  
sounding_dim,  
level_dim  
hPa  
Pressure levels

**pressure_weight**  
float  
sounding_dim,  
layer_dim  
Layer dependent weights needed to apply the averaging kernels

**xch4**  
float  
sounding_dim  
1e-9  
Retrieved column dry-air mole fraction of atmospheric methane (XCH4) in ppb

**xch4_uncertainty**  
float  
sounding_dim  
1e-9  
1-sigma (scaled) uncertainty of the retrieved column-average dry-air mole fraction of atmospheric methane

**xch4_averaging_kernel**  
float  
sounding_dim,  
layer_dim  
Normalized column averaging kernel

**ch4_profile_apriori**  
float  
sounding_dim,  
layer_dim  
1e-9  
A priori dry-air mole fraction profile of atmospheric methane

**xch4_quality_flag**  
int  
sounding_dim  
Quality flag for XCH4 retrieval, 0 = good, 1 = bad

XCH4 via RemoTeC from GOSAT2 (CH4_GO2_SRPR) for the Essential Climate Variable (ECV) Greenhouse Gases (GHG)
<table>
<thead>
<tr>
<th>Variable</th>
<th>Type</th>
<th>Dimensions</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>l1b_name</td>
<td>char</td>
<td>sounding_dim, char_l1bname</td>
<td>Name of the Level 1B file of the sounding</td>
</tr>
<tr>
<td>signal_to_noise_window</td>
<td>float</td>
<td>sounding_dim, window_dim, polarization_dim</td>
<td>Signal to noise ratio per retrieval window and for both polarization directions</td>
</tr>
<tr>
<td>dry_airmass_layer</td>
<td>float</td>
<td>sounding_dim, layer_dim</td>
<td>Dry airmass per layer</td>
</tr>
<tr>
<td>altitude</td>
<td>float</td>
<td>sounding_dim</td>
<td>Vertical altitude above the surface</td>
</tr>
<tr>
<td>air_temperature</td>
<td>float</td>
<td>sounding_dim, level_dim</td>
<td>The bulk temperature of the air at each level</td>
</tr>
<tr>
<td>surface_altitude_stdev</td>
<td>float</td>
<td>sounding_dim</td>
<td>Standard deviation of the surface elevation within the sounding</td>
</tr>
<tr>
<td>x_wind</td>
<td>float</td>
<td>sounding_dim, level_dim</td>
<td>Eastward wind velocity</td>
</tr>
<tr>
<td>y_wind</td>
<td>float</td>
<td>sounding_dim, level_dim</td>
<td>Northward wind velocity</td>
</tr>
<tr>
<td>chi2</td>
<td>float</td>
<td>sounding_dim</td>
<td>Chi-squared value of the sounding</td>
</tr>
<tr>
<td>optical_thickness_of_atmosphere_layer_due_to_ambient_aerosol</td>
<td>float</td>
<td>sounding_dim, window_dim</td>
<td>Scattering optical thickness per retrieval window</td>
</tr>
<tr>
<td>raw_xch4_err</td>
<td>float</td>
<td>sounding_dim</td>
<td>1-sigma (unscaled) statistical uncertainty of the retrieved column-average dry-air mole fraction of atmospheric methane</td>
</tr>
<tr>
<td>h2o_column_1593</td>
<td>float</td>
<td>sounding_dim</td>
<td>Retrieved total water column at 1593 nm</td>
</tr>
<tr>
<td>h2o_column_1629</td>
<td>float</td>
<td>sounding_dim</td>
<td>Retrieved total water column at 1629 nm</td>
</tr>
<tr>
<td>h2o_column_2042</td>
<td>float</td>
<td>sounding_dim</td>
<td>Retrieved total water column at 2042 nm</td>
</tr>
<tr>
<td>surface_albedo_758</td>
<td>float</td>
<td>sounding_dim</td>
<td>The retrieved albedo at 758 nm</td>
</tr>
<tr>
<td>surface_albedo_1593</td>
<td>float</td>
<td>sounding_dim</td>
<td>The retrieved albedo at 1593 nm</td>
</tr>
<tr>
<td>surface_albedo_1629</td>
<td>float</td>
<td>sounding_dim</td>
<td>The retrieved albedo at 1629 nm</td>
</tr>
<tr>
<td>surface_albedo_2042</td>
<td>float</td>
<td>sounding_dim</td>
<td>The retrieved albedo at 2042 nm</td>
</tr>
<tr>
<td>intensity_offset_o2a</td>
<td>float</td>
<td>sounding_dim</td>
<td>The retrieved intensity offset in the O2A band</td>
</tr>
</tbody>
</table>
### Parameter List

<table>
<thead>
<tr>
<th>Parameter Name</th>
<th>Type</th>
<th>Dim</th>
<th>Unit</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>intensity_offset_band_2</td>
<td>float</td>
<td>sounding_dim</td>
<td>W cm(^{-2})</td>
<td>The retrieved intensity offset in spectral window 2</td>
</tr>
<tr>
<td>intensity_offset_band_3</td>
<td>float</td>
<td>sounding_dim</td>
<td>W cm(^{-2})</td>
<td>The retrieved intensity offset in spectral window 3</td>
</tr>
<tr>
<td>intensity_offset_band_4</td>
<td>float</td>
<td>sounding_dim</td>
<td>W cm(^{-2})</td>
<td>The retrieved intensity offset in spectral window 4</td>
</tr>
<tr>
<td>raw_xch4</td>
<td>float</td>
<td>sounding_dim</td>
<td>1e(^{-9})</td>
<td>Retrieved column dry-air mole fraction of atmospheric methane (XCH4) in ppb before scattering correction</td>
</tr>
<tr>
<td>xch4_no_bias_correction</td>
<td>float</td>
<td>sounding_dim</td>
<td>1e(^{-9})</td>
<td>Retrieved column dry-air mole fraction of atmospheric methane (XCH4) in ppb before bias correction</td>
</tr>
<tr>
<td>raw_xco2</td>
<td>float</td>
<td>sounding_dim</td>
<td>1e(^{-6})</td>
<td>Retrieved column dry-air mole fraction of atmospheric carbon dioxide (XCO2) in ppm before scattering correction</td>
</tr>
<tr>
<td>xco2_apriori</td>
<td>float</td>
<td>sounding_dim</td>
<td>1e(^{-6})</td>
<td>A priori dry-air mole fraction of atmospheric carbon dioxide</td>
</tr>
<tr>
<td>co2_profile_apriori</td>
<td>float</td>
<td>sounding_dim, layer_dim</td>
<td>1e(^{-6})</td>
<td>A priori dry-air mole fraction profile of atmospheric carbon dioxide</td>
</tr>
<tr>
<td>xco2_averaging_kernel</td>
<td>float</td>
<td>sounding_dim, layer_dim</td>
<td></td>
<td>Normalized column averaging kernel for carbon dioxide</td>
</tr>
<tr>
<td>raw_xco2_err</td>
<td>float</td>
<td>sounding_dim</td>
<td>1e(^{-6})</td>
<td>1-sigma (unscaled) statistical uncertainty of the retrieved column-average dry-air mole fraction of atmospheric carbon dioxide</td>
</tr>
</tbody>
</table>
5.2 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: retrievals for normal or sunglint data, 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 < 7.
- SNR > 50.
- Standard deviation of surface elevation within GOSAT-2 ground pixel should be < 150 m
- SZA < 75$^\circ$.
- 0.98 < CO2 (1.6 micron) / CO2 (2.0 micron) < 1.15
- 0.88 < O2 (retrieved) / O2 (prior) < 1.035
- 0.9 < H2O (1.6 micron) / H2O (2.0 micron) < 1.5
5.3 Recommended data usage

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

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

If the data are to be compared with other XCO₂ and/or XCH₄ data for which vertical profile information is available (e.g. inverse modeling, comparison to models, comparison to measured profiles), the column averaging kernels should be used. Here it should be noted that the column averaging kernels are to be applied to layer sub-columns (m-2), as these are the quantities directly retrieved in the RemoTeC algorithm. For model comparisons the retrieved XCO₂ should be compared to \([VCO₂]_{\text{model}}/[\text{VAIR}]_{\text{model}}\) where \([\text{VAIR}]_{\text{model}}\) is the total dry air column provided by the model and \([VCO₂]_{\text{model}}\) is the model total CO₂ column after applying the column averaging kernel, viz.:

\[
[VCO₂]_{\text{model}} = [VCO₂]_{\text{prior}} + a^T(x_{\text{model}} - x_{\text{prior}})
\]

where \([VCO₂]_{\text{prior}}\) is the prior CO₂ total column used in the retrieval, \(x_{\text{model}}\) is the vertical CO₂ profile from the model (as sub-columns) and \(x_{\text{prior}}\) 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.

5.4 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).
6. References


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