Product User Guide and Specification (PUGS) – ANNEX B for products CO2_GOS_SRFP, CH4_GOS_SRFP (v2.3.8, 2009-2018)

C3S_312b_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	Update for CDR2 (2009-2017)	All
3.0	12-August-2019	Update for CDR3 (2009-2018)	All
3.1	03-November-2019	Update after review by Assimila: Correction of typos.	All

Related documents

Reference ID	Document
D1	Main PUGS: Buchwitz, M., et al., Product User Guide and Specification (PUGS) – Main document for Greenhouse Gas (GHG: CO2 & CH4) data set CDR 3 (2003-2018), project C3S_312b_Lot2_DLR – Atmosphere, 3.1, 2019. *(this document is an ANNEX to the Main PUGS)*

Acronyms

Acronym	Definition
ATBD	Algorithm Theoretical Basis Document
CAR	Climate Assessment Report
C3S	Copernicus Climate Change Service
CCI	Climate Change Initiative
CDR	Climate Data Record
CDS	(Copernicus) Climate Data Store
CRG	Climate Research Group
D/B	Data base
EC	European Commission
ECMWF	European Centre for Medium Range Weather Forecasting
ECV	Essential Climate Variable
EO	Earth Observation
ESA	European Space Agency
EU	European Union
EUMETSAT	European Organisation for the Exploitation of Meteorological Satellites
FP	Full Physics retrieval method
FTIR	Fourier Transform InfraRed
FTS	Fourier Transform Spectrometer
GCOS	Global Climate Observing System
GEOSS	Global Earth Observation System of Systems
GHG	GreenHouse Gas
GOSAT	Greenhouse Gases Observing Satellite
IPCC	International Panel in Climate Change
IUP	Institute of Environmental Physics (IUP) of the University of Bremen, Germany
JAXA	Japan Aerospace Exploration Agency
KIT	Karlsruhe Institute of Technology
L1	Level 1
L2	Level 2
L3	Level 3
L4	Level 4
LMD	Laboratoire de Météorologie Dynamique
MACC	Monitoring Atmospheric Composition and Climate, EU GMES project
NA	Not applicable
NetCDF	Network Common Data Format
NIES	National Institute for Environmental Studies
NIR	Near Infra Red

NOAA	National Oceanic and Atmospheric Administration
Obs4MIPs	Observations for Climate Model Intercomparisons
ppb	Parts per billion
ppm	Parts per million
PR	(light path) PRoxy retrieval method
PVIR	Product Validation and Intercomparison Report
QA	Quality Assurance
QC	Quality Control
REQ	Requirement
RMS	Root-Mean-Square
RTM	Radiative transfer model
SNR	Signal-to-Noise Ratio
SRON	SRON Netherlands Institute for Space Research
SWIR	Short Wave Infra Red
SZA	Solar Zenith Angle
TANSO	Thermal And Near infrared Sensor for carbon Observation
TANSO-FTS	Fourier Transform Spectrometer on GOSAT
TBC	To be confirmed
TBD	To be defined / to be determined
TCCON	Total Carbon Column Observing Network
TIR	Thermal Infra Red
TR	Target Requirements
TRD	Target Requirements Document
URD	User Requirements Document
WMO	World Meteorological Organization
Y2Y	Year-to-year (bias variability)

General definitions

Table 1 lists some general definitions relevant for this document.

Table 1: General definitions.

Item	Definition
XCO_2	Column-averaged dry-air mixing ratios (mole fractions) of CO_2
XCH_4	Column-averaged dry-air mixing ratios (mole fractions) of CH_4
L1	Level 1 satellite data product: geolocated radiance (spectra)
L2	Level 2 satellite-derived data product: Here: CO_2 and CH_4 information for each ground-pixel
L3	Level 3 satellite-derived data product: Here: Gridded CO_2 and CH_4 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_2 and CH_4

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 C3S_312b_Lot2.

Within this project satellite-derived atmospheric carbon dioxide (CO_2) and methane (CH_4) 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 GHG satellite-derived data products are:

- Column-averaged dry-air mixing ratios (mole fractions) of CO_2 and CH_4, denoted XCO_2 (in parts per million, ppm) and XCH_4 (in parts per billion, ppb), respectively.
- Mid/upper tropospheric mixing ratios of CO_2 (in ppm) and CH_4 (in ppb).

This document describes the C3S products CO2_GOS_SRFP and CH4_GOS_SRFP.

These products are XCO_2 and XCH_4 Level 2 products as retrieved from GOSAT using algorithms developed at SRON, The Netherlands.

Executive summary

This document is the annex B of the Product User Guide (PUG), which is a deliverable of the C3S project. This document describes the RemoteC XCO_2 and XCH_4 Full Physics data products (CO2_GOS_SRFP and CH4_GOS_SRFP) so that it will be clear for the user how to use the product. The description includes quality flags and metadata, data format, product grid, known limitations, bias correction, and the product (column) averaging kernels and a description how to use them.

1. Data product description

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_2 and CH_4 from its SWIR bands, *Yoshida et al., 2010*. It is equipped with two instruments, the Thermal And Near Infrared Sensor for carbon Observations - Fourier Transform Spectrometer (TANSO-FTS) as well as a dedicated Cloud and Aerosol Imager (TANSO-CAI).

The TANSO-FTS instrument has four spectral bands with a high spectral resolution 0.3 cm^{-1}, 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.

The measurement strategy of TANSO-FTS is optimized for the characterization of continental-scale sources and sinks. TANSO-FTS utilizes 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 3 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 the surface reflectance is high, TANSO-FTS also observes in sunglint mode over the ocean within ±20° of the sub-solar latitude.

The CH4_GOS_SRFP and CO2_GOS_SRFP products are retrieved from GOSAT TANSO-FTS NIR and SWIR spectra using the RemoTeC algorithm that is being 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 CH4 band at 1.64 µm. Within the retrieval procedure the sub-columns of CO_2 and CH_4 in different altitude layers are being retrieved. To obtain the column averaged dry air mixing ratios XCO2 and XCH4 the sub-columns are summed up to get the total column which is divided by the dry-air columns obtained from ECMWF model data in combination with a surface elevation data base. The retrieved XCH4 and XCO2 have been extensively validated with ground based TCCON measurements. To further improve accuracy a bias correction has been developed based on TCCON comparisons. We use the GGG2014 TCCON dataset, *Wunch et al., 2015*.

More details on the technical aspects of the retrievals can be found in the ATBD Annex-B.

Figure 1: Global XCO_2 for the 2009-2018 period for the CO2_GOS_SRFP product on a 1 by 1 degree resolution.

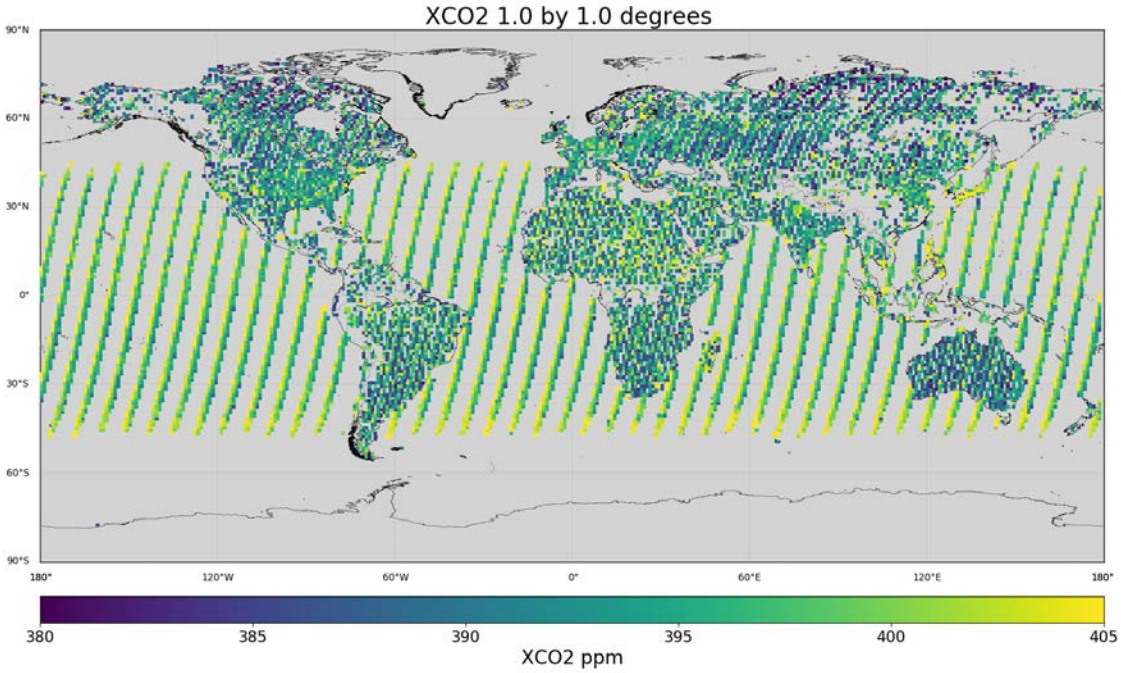
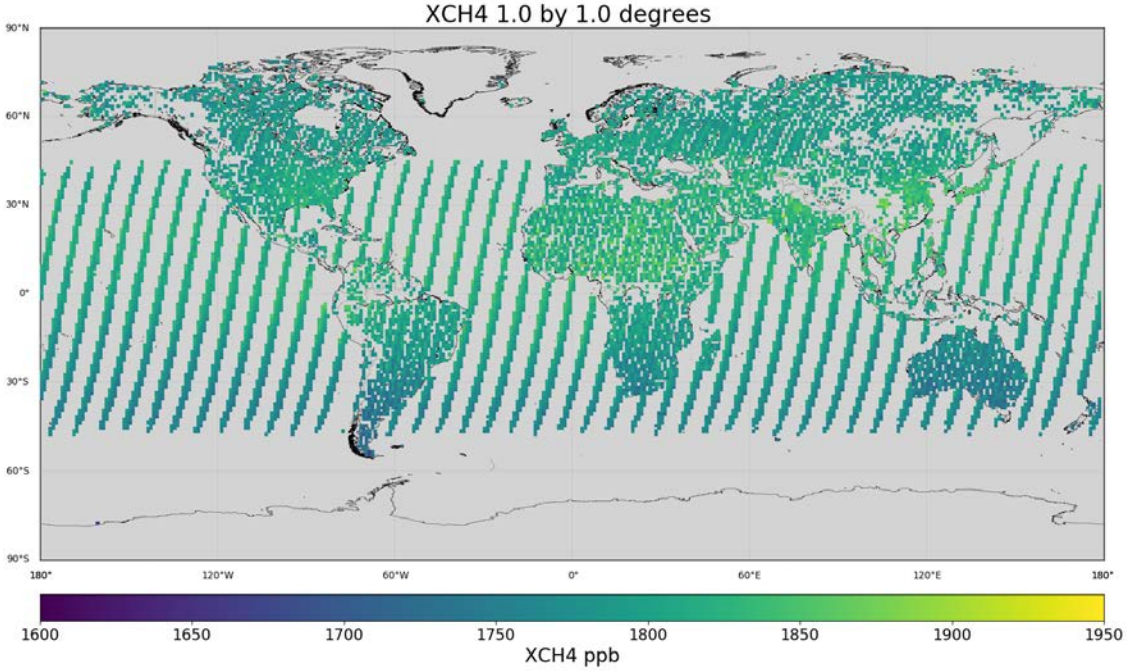


Figure 2: Global XCH_4 for the 2009-2018 period for the CH4_GOS_SRFP product on a 1 by 1 degree resolution.



2. Target requirements

Table 1: Target requirements for XCH_4 and XCO_2

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 #))

Table 1 shows the target requirements for XCH_4 and XCO_2 (Threshold, Breakthrough and Goal) as derived in the Target Requirements Document (TRD).

3. Data usage information

3.1 Product Content and Format

The CH4_GOS_SRFP and CO2_GOS_SRFP data products are stored per day in a single NetCDF file. Retrieval results are provided for the individual GOSAT spatial footprints, i.e. no averaging has been applied. The product file contains the key standard products, i.e. the retrieved column averaged dry air mixing ratios XCO2 and XCH4 with bias correction, averaging kernels and quality flags, as well as secondary products specific for the RemoTeC algorithm.

Table 2: Common variables for the CO2_GOS_SRFP product

Name	Type	Dim.	Units	Description
solar_zenith_angle	float	n	degrees	Angle between line of sight to the sun and local vertical
sensor_zenith_angle	float	n	degrees	Angle between the line of sight to the sensor and the local vertical
time	float	n	seconds	Seconds since 1970-01-01 00:00:00
longitude	float	n	degrees_east	Center longitude
latitude	float	n	degrees_north	Center latitude
pressure_levels	float	n, 13	hPa	Pressure levels
pressure_weight	float	n, 12		Layer dependent weights needed to apply the averaging kernels
xco2	float	n	1e-6	Retrieved column dry-air mole fraction of atmospheric carbon dioxide (XCO2) in ppm
xco2_uncertainty	float	n	1e-6	1-sigma uncertainty of the retrieved column-average dry-air mole fraction of atmospheric carbon dioxide
xco2_averaging_kernel	float	n, 12		Normalized column averaging kernel
co2_profile_apriori	float	n, 12	1e-6	A priori dry-air mole fraction profile of atmospheric carbon dioxide
xco2_quality_flag	int	n		Quality flag for XCO2 retrieval, 0 = good, 1 = bad

Table 2: Product specific (additional) variables for the CO2_GOS_SRFP product

Name	Type	Dim.	Units	Description
flag_landtype	int	n		0 = land, 1 = ocean
flag_sunglint	int	n		0 = no sunglint, 1 = sunglint
gain	char	n		gain setting of sensor, H = gain H, M = gain M
exposure_id	int	n		Exposure identification number of the sounding
l1b_name	char	n, 44		Name of the Level 1B file of the sounding
signal_to_noise_window	float	n, 4, 2		Signal to noise ratio per retrieval window and for both polarization directions
dry_airmass_layer	float	n, 12	m-2	Dry airmass per layer
altitude	float	n	m	Vertical distance above the surface
air_temperature	float	n, 13	K	The bulk temperature of the air at each level
surface_elevation_stdev	float	n	m	Standard deviation of the surface elevation within the sounding
x_wind	float	n, 13	m s-1	Eastward wind velocity
y_wind	float	n, 13	m s-1	Northward wind velocity
chi2	float	n		Chi-squared value of the sounding
optical_thickness_of_atmosphere_layer_due_to_ambient_aerosol	float	n, 4		Scattering optical thickness per retrieval window
raw_xco2	float	n	1e-6	Retrieved column dry-air mole fraction of atmospheric carbon dioxide (XCO2) in ppm before bias correction
raw_xco2_err	float	n	1e-6	1-sigma statistical uncertainty of the retrieved column-average dry-air mole fraction of atmospheric carbon dioxide
h2o_column	float	n	m-2	Retrieved total water column
surface_albedo_758	float	n		The retrieved albedo at 758 nm
surface_albedo_1593	float	n		The retrieved albedo at 1593 nm
surface_albedo_1629	float	n		The retrieved albedo at 1629 nm
surface_albedo_2042	float	n		The retrieved albedo at 2042 nm
intensity_offset_o2a	float	n	W cm-2	The retrieved intensity offset in the O2A band
aerosol_size	float	n		Retrieved size parameter of the aerosol distribution
aerosol_central_height	float	n	m	Peak height of the aerosol Gaussian height distribution
aerosol_total_column	float	n	m-2	Retrieved total aerosol column

Table 4: Common variables for the CH4_GOS_SRFP product

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

Table 5: Product specific (additional) variables for the CH4_GOS_SRFP product

Name	Type	Dim.	Units	Description
flag_landtype	int	n		0 = land, 1 = ocean
flag_sunglint	int	n		0 = no sunglint, 1 = sunglint
gain	char	n		gain setting of sensor, H = gain H, M = gain M
exposure_id	int	n		Exposure identification number of the sounding
l1b_name	char	n, 44		Name of the Level 1B file of the sounding
signal_to_noise_window	float	n, 4, 2		Signal to noise ratio per retrieval window and for both polarization directions
dry_airmass_layer	float	n, 12	m-2	Dry airmass per layer
altitude	float	n	m	Vertical altitude above the surface
air_temperature	float	n, 13	K	The bulk temperature of the air at each level
surface_altitude_stdev	float	n	m	Standard deviation of the surface elevation within the sounding
x_wind	float	n, 13	m s-1	Eastward wind velocity
y_wind	float	n, 13	m s-1	Northward wind velocity
chi2	float	n		Chi-squared value of the sounding
optical_thickness_of_atmosphere_layer_due_to_ambient_aerosol	float	n, 4		Scattering optical thickness per retrieval window
raw_xch4	float	n	1e-9	Retrieved column dry-air mole fraction of atmospheric methane (XCH4) in ppb before bias correction
raw_xch4_err	float	n	1e-9	1-sigma statistical uncertainty of the retrieved column-average dry-air mole fraction of atmospheric methane
h2o_column	float	n	m-2	Retrieved total water column
surface_albedo_758	float	n		The retrieved albedo at 758 nm
surface_albedo_1593	float	n		The retrieved albedo at 1593 nm
surface_albedo_1629	float	n		The retrieved albedo at 1629 nm
surface_albedo_2042	float	n		The retrieved albedo at 2042 nm
intensity_offset_o2a	float	n	W cm-2	The retrieved intensity offset in the O2A band
aerosol_size	float	n		Retrieved size parameter of the aerosol distribution
aerosol_central_height	float	n	m	Peak height of the aerosol Gaussian height distribution
aerosol_total_column	float	n	m-2	Retrieved total aerosol column

3.2 Quality Flags and Metadata

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

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

- Error on retrieved XCO2 < 1.2 ppm
- $\chi 2$ of fit < 4.5
- $\chi 2$ of fit in O2A-band < 4
- SNR > 50
- Standard deviation of surface elevation within GOSAT ground pixel should be < 80 m
- 0 < aerosol_filter < 300
- Aerosol Optical Thickness < 0.3
- 3 < Aero_size < 5
- SZA < 70^o
- -1e-9 < Intensity Offset O2A-band < 3e-9
- Blended Albedo < 0.9
- 0.99 < CO2 (1.6 micron) / CO2 (2.0 micron) < 1.015
- 0.95 < O2 (retrieved) / O2 (prior) < 1.02
- 0.95 < H2O (1.6 micron) / H2O (2.0 micron) < 1.08

For **gain M**:

- Number of iteration steps in retrieval < 25
- Error on retrieved XCO2 < 1.2 ppm
- $\chi 2$ of fit < 5

- $\chi 2$ of fit in O2A-band < 4
- $\chi 2$ of fit in window 2 < 4
- SNR > 50
- Standard deviation of surface elevation within GOSAT ground pixel should be < 80 m
- 0 < aerosol_filter < 350
- Aerosol Optical Thickness < 0.25
- 3 < Aero_size < 4
- SZA < 70^{o}
- 0.99 < CO2 (1.6 micron) / CO2 (2.0 micron) < 1.015
- 0.97 < O2 (retrieved) / O2 (prior) < 1.01
- 0.95 < H2O (1.6 micron) / H2O (2.0 micron) < 1.05

For **sunglint**:

- Number of iteration steps in retrieval < 31
- Cirrus Signal < 8e-10
- $\chi 2$ of fit < 4
- $\chi 2$ of fit in O2A-band < 4
- $\chi 2$ of fit in window 4 < 10
- -1e-5 < Retrieved slope of albedo in window 4 < 5e-5
- -1e-9 < Intensity Offset O2A-band < 3e-9
- 0.99 < CO2 (1.6 micron) / CO2 (2.0 micron) < 1.01
- 0.965 < O2 (retrieved) / O2 (prior) < 1.00
- 0.95 < H2O (1.6 micron) / H2O (2.0 micron) < 1.05

3.3 Bias Correction

From comparison with TCCON it was found that the error in XCO2 correlates with the solar zenith angle (sza) and the aerosol filter ϕ. Based on this correlation the following bias correction has been developed for XCO2 for **gain H**:

$$XCO2_{corr} = XCO2 * (a + b * \phi + c * sza)$$

with a = 0.999995, b = 2.8204e-5, c = 7.287e-5.
For **gain M** we apply a correction based on just the aerosol filter ϕ:

$$XCO2_{corr} = XCO2 * (a + b * \phi)$$

and with a= 1.004228, b = -3.00868e-6.
For **sunglint** data we use a correction factor based on the O2 ratio:

$$XCO2_{corr} = XCO2 * (a + b * RO2)$$

with a = 1.283633 and b = -0.28368.
The bias correction parameters are obtained from fits to the GOSAT-TCCON differences.

Similarly, for XCH4 it was found that the error in XCH4 correlates with the solar zenith angle (sza) and the aerosol filter ϕ. Based on this correlation the following bias correction has been developed for XCH4 for **gain H**:

$$XCH4_{corr} = XCH4 * (a + b * \phi + c * sza)$$

with a = 0.996226, b = 4.4482e-5, c = 6.0089e-5.
For **gain M** we apply a correction based on just the aerosol filter ϕ:

$$XCH4_{corr} = XCH4 * (a + b * \phi)$$

with a= 1.002728, b = 1.0053e-5.
For **sunglint** data we use a correction factor based on the O2 ratio:

$$XCH4_{corr} = XCH4 * (a + b * RO2)$$

with a = 1.18122 and b = -0.18569.
The bias correction parameters are obtained from fits to the GOSAT-TCCON differences.

Figure 3: Co-located GOSAT-TCCON XCH4 measurements for gain H measurements

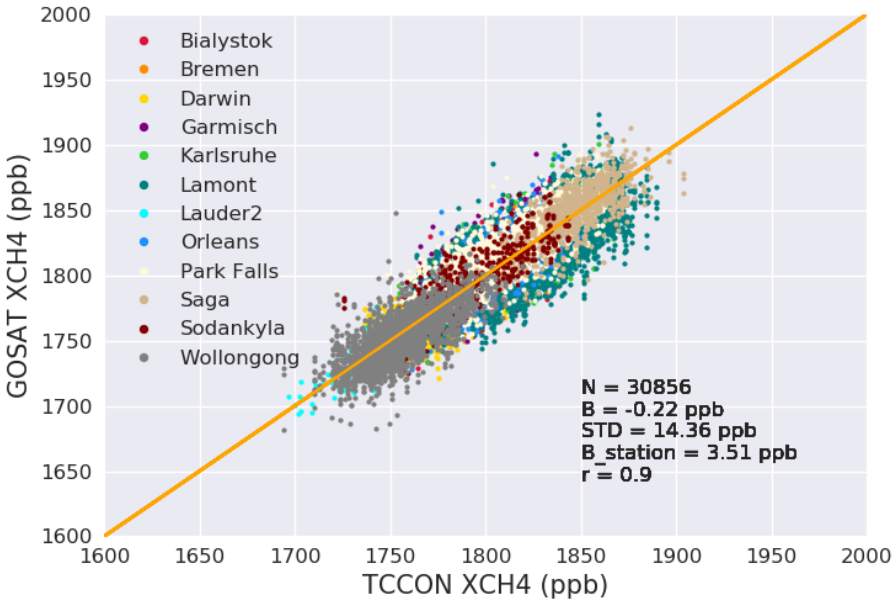
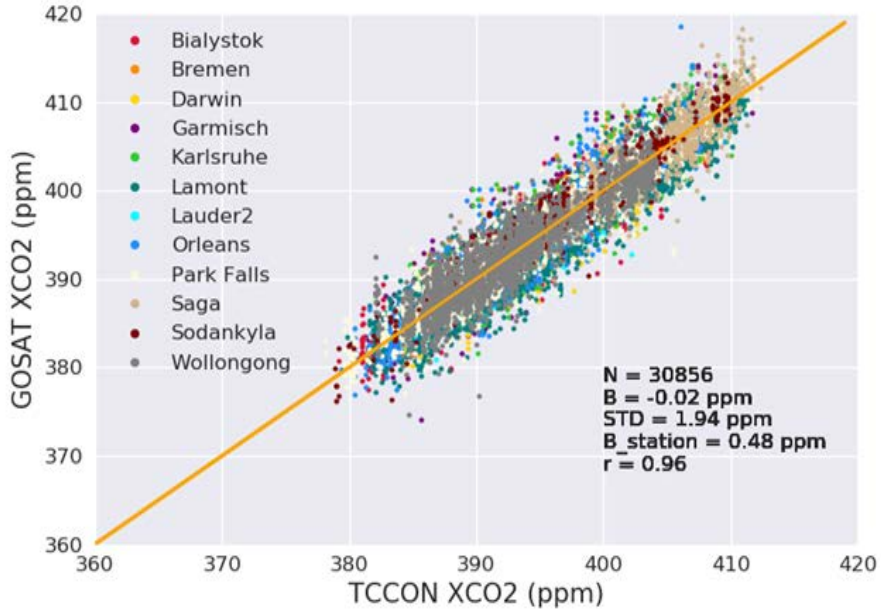


Figure 4: Co-located GOSAT-TCCON XCO2 measurements for gain H measurements



3.4 Recommended data usage

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

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

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

For model comparisons the retrieved XCO2 should be compared to $[VCO2]'_{model}/[VAIR]_{model}$ where $[VAIR]_{model}$ is the total dry air column provided by the model and $[VCO2]'_{model}$ is the model total CO2 column after applying the column averaging kernel, viz.:

$$[VCO2]'_{model} = [VCO2]_{prior} + \mathbf{a}^T(\mathbf{x}_{model} - \mathbf{x}_{prior})$$

where $[VCO2]_{prior}$ is the prior CO total column used in the retrieval, $\mathbf{x}_{model}$ is the vertical CO2 profile from the model (as sub-columns) and $\mathbf{x}_{prior}$ is the prior vertical profile from the retrieval. For application of the column averaging kernel the model vertical profile should be re-calculated on the vertical grid of the retrieval (preferred) or the averaging kernel has to be interpolated to the vertical grid of the model. This procedure holds in the same way for the SRFP XCH4 product, but then replacing all instances of CO2 with CH4.

3.4 Tools for Reading the Data

The data are stored in Netcdf format which can be read with standard tools in the common programming languages (IDL, Matlab, Python, Fortran90, C++, etc).

3.5 Known Limitations and Issues

- The data retrieved for the **H-gain** instrument settings are considered highest quality and are well validated. In the "raw" retrievals (i.e. before bias correction) there is a bias between **H-gain** and **sunglint** and **M-gain** retrievals, respectively. Although these biases have been corrected in the bias-corrected products, there may still be a small residual bias left, especially due to the limited number of validation sites for **sunglint** and **M-gain** retrievals.
- The 2nd half of December 2014 and the whole of January 2015 have no data due to the GOSAT satellite being in calibration mode after switching to the backup pointing system.

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