ESA Climate Change Initiative "Plus" (CCI+)

End-to-End ECV Uncertainty Budget (E3UB) Version 3.0
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For the RemoTeC XCH4 GOSAT-2 SRON Full-Physics Product (CH4_GO2_SRFP) Version 2.0.0

for the Essential Climate Variable (ECV)

Greenhouse Gases (GHG)

Written by:

GHG-CCI+ project team

Lead author:

Trismono Candra Krisna

(SRON Netherlands Institute for Space Research, Utrecht, The Netherlands)

Co-authors:

Ilse Aben, Lianghai Wu, Otto Hasekamp, Jochen Landgraf

(SRON Netherlands Institute for Space Research, Utrecht, The Netherlands)

Change log

Version Nr.	Date	Status	Reason for change
Version 1	27. Oct. 2020	Draft	New document
Version 1.1	4. Jan. 2021	As submitted	- Definition uncertainty ratio - Update format - Remove typos
Version 1.1	4. Feb. 2021	As submitted	- Update after ESA reviews - Remove typos
Version 2.0	04. Nov. 2021	As submitted	- Updated to version 2.0.0
Version 3.0	27. Jan. 2022	As submitted	- Updated doc to version 3.0

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Executive summary

This report summarizes the performance of the RemoTeC GOSAT-2 SRFP XCH_4 retrieval. In general, we find very good agreement with TCCON and GOSAT-1 data for the two modes (normal and sunglint). The mean bias (global offset) is 0.1 ppb with a single measurement precision of 14.4 ppb. The spatial accuracy (standard deviation site biases) is 2.4 ppb and mean standard deviation of around 13.0 ppb is observed for most TCCON stations. Based on comparison with TCCON we scale the retrieved statistical error by a factor 1.44 for normal mode and 1.38 for sunglint mode to obtain a representative random error. This corresponds to an uncertainty ratio of 0.69 for normal mode and 0.72 for sunglint mode.

Correlations of the observed bias with retrieved parameters were also checked. It was found that after the initial bias correction based on the retrieved albedo of Band 2, similar to the bias correction used for GOSAT-1, the remaining correlations were small.

Estimates of achieved data quality: CH4_GO2_SRFP					
Sensor	**Algorithm**	**Single measurement precision (1-sigma) in [ppb]**	**Mean bias (global offset) [ppb]**	**Spatial Accuracy: Relative systematic error [ppb]**	**Uncertainty ratio (scaling)**
TANSO-FTS-2 on GOSAT-2	SRFP v1.0.0 (RemoTeC)	14.4	0.1	2.4	0.69 (0.72 glint)

Table 1: An overview of the achieved data quality for the XCH_4 SRFP product.

1 Introduction

1.1 Purpose of document

This E3UB provides an overview of random and systematic errors affecting the SRON SRFP XCH_4 retrieval submitted for the ESA GHG-CCI+ Climate Research Data Package version 1, in October 2020. Application of confidence limits to the retrieval is required to translate remotely sensed data presented here into modelled estimations with a known degree of confidence, allowing detection of climate change impacts additional to the natural variability of greenhouse gases. In particular, the GHG-CCI+ User Requirements have placed strict measurement accuracy and precision requirements on the participating GHG retrievals, allowing identification of minute changes in magnitude and sign of XCH_4 concentration change (Buchwitz et al., 2011; 2014).

1.2 Intended audience

This document is intended for users in the modelling community applying the SRFP XCH_4 product for CO_2 inversions, as well as remote sensing experts interested in atmospheric soundings of XCH_4. In both cases the work presented here will give the user a more thorough understanding of error implicit in this GHG-CCI+ product.

1.3 Error term definitions

Error terms used in this report are defined to maintain consistency with other CCI+ user group error terms recommended at the 2014 CCI co-location meeting. Following the descriptions of Wagner et al. (2012):

Error	Difference between measured values and reality (residual of a measurement's accuracy).
Uncertainty	Degree of confidence in the range of a measured value's truth (standard deviation).
Absolute accuracy	Proximity of remotely sensed measurement to in-situ measurement, assuming the in-situ measurement is able to provide a best estimate of observed quantity. Absolute accuracy reflects the best effort of the remote sensing system at reproducing the real-world value by incorporating all random and systematic errors affecting the retrieval.

Relative accuracy	Ratio between the instrument’s calibration standard (the best possible measurement the instrument is able to make) against the instrument characteristics at the time of measurement.
Precision	Repeatability of a measurement.

2 Error sources

The majority of error is added to measurements from sources grouped into two themes – scattering of radiation into and out of the sensed light path by poorly quantified aerosol loading, cloud, surface reflectivity and meteorological parameters (temperature, pressure and humidity); and instrumental uncertainties (cross section and solar model inaccuracy, system noise and measurement resolution of instrument components) (Connor et al., 2008, Boesch et al., 2011). In addition to single measurement error, issues of correlation lengths are introduced when the retrievals are used for subsequent generation of level 3 products (Buchwitz et al., 2014; Chevalier et al., 2014). The aforementioned errors can be further grouped into systematic – those which remain stable across measurement series; and random error components – noise in the system induced by unexpected and / or unaccounted for stimuli.

2.1 Systematic

Systematic retrieval errors include algorithmic effects such as inaccuracy in the solar and radiative transfer models, which will not change with the duration of the satellite's sensing. The same applies to restrictions in instrument calibration accuracy, for instance modelling of the instrument line shape, which remains fixed following launch (although is modifiable when enough information on ILS degradation is built up). Viewing geometry also affects retrievals in a regular fashion by modifying the light path of sensed radiation as a function of the instrument and Sun's position, however interplay between increased path lengths and random error components such as aerosol optical depth add complications to issue of measurement geometry. A-priori error added to XCO_2 and XCH_4 measurements occurs when the retrieval ingests inaccurate input data from models and databases of surface reflectivity, surface pressure, vertical pressure grids, humidity profiles and a-priori CO_2 and CH_4 profiles.

2.2 Random

Random errors are introduced to observations at the sensing stage of a measurement by detector noise, although to a certain extent this error parameter can be estimated as a function of detector component signal to noise ratios during instrument calibration. Far more significantly, atmospheric parameters are able to have major effects on sounding measurements by scattering light in and out of the sensed column. Errors due to unknown aerosol parameters are particularly pronounced where the scattering and absorption effects of suspended particulate matter are poorly modelled, as they inevitably will be when accounting for a tiny subset of all aerosol sizes, morphology and composition. Scattering due to high, optically thin clouds that are not screened from observation record present similar problems.

3 Methodology

3.1 SRON SRFP

The CH4_GO2_SRFP product is retrieved from GOSAT-2 TANSO-FTS SWIR spectra using the RemoTeC algorithm that has been jointly developed at SRON and KIT (Butz et al., 2009; Butz et al., 2010; Butz et al., 2011; Schepers et al., 2012). 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 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-SRFP document **(**ATBD 2020**)**.

3.2 Comparison to GOSAT-1 SRFP

The GOSAT-1 SRFP retrieval (CH4_GOS_SRFP product) has been extensively validated and offers an excellent opportunity for comparison. As the GOSAT-1 product reports both bias corrected and non-bias corrected values we will compare both the bias corrected and non-bias corrected GOSAT-2 values. The period covered is February 2019 – August 2019 as for GOSAT-1 only the period up to August 2019 is available. We split the GOSAT-2 observations into glint and non-glint ("land") sets and compare them separately. As both satellites observe at similar overpass times, we will co-locate the GOSAT and GOSAT-2 footprints spatially by classing them into 2°x2° boxes and temporally by matching the overpasses by day. All groupings are then averaged to create daily averaged 2°x2° values. Any GOSAT-2 grouping that does not have a corresponding match for GOSAT-1 is discarded.

At the time of writing there were not enough TCCON sites with data for validation of the Glint observations. The GOSAT-2 glint observations have therefor been validated and bias corrected using the GOSAT-1 bias corrected product (CH4_GOS_SRFP). Observations are matched more closely by only comparing the individual footprints that match closest within 0.5 degrees for each day, which is typically within the hour.

3.3 TCCON

The Total Carbon Column Observing Network (TCCON) is a global network of Fourier transform spectrometers built for the purpose of validating space-borne measurements of

XCO_2 and XCH_4 (Wunch et al., 2015). TCCON observes these gases with a precision on mole fractions of ~0.15% and ~0.2% for CO_2 and CH_4 respectively (Toon et al., 2009). Although providing highly accurate measurements, the sparseness of the TCCON sites presents a challenge for validation; offering precise GHG measurements for only a limited range of geographic and meteorological conditions.

Additional considerations should be made when validating with TCCON data for differing sensitivity of instruments between TCCON and the satellite instrument, reflected in a-priori information used for each retrieval. Removing the influence of the retrieval a-priori, and replacing with the TCCON a-priori allows for a fairer comparison between the two datasets, although slight differences in retrieval methodologies prevent a 1:1 comparison. Users of GHG-CCI+ data (particularly in the modelling community) should note that the published CCI+ products are not corrected with TCCON a-priori information (due to a-priori differences between sites), and so will find slightly worse correlations between satellite retrieved GHGs and TCCON values in their own comparisons.

TCCON data used for error assessments come from the GGG2014 collection (available from http://tccon.ornl.gov/).

3.4 Co-location

To assess the quality of SRFP retrieval XCH_4 observations against rigorously validated ground based TCCON values, SRFP soundings are matched to TCCON observations spatially and temporally. The process of matching these two data sources is referred to as co-location. Below we detail the SRON co-location techniques, whose methodology has a bearing on subsequent error statistics.

Spatial

We follow a straightforward approach by using a box ±2.5°in latitude and longitude around every TCCON station. In previous GOSAT-1 reports **(**CECR2017; C3SPQAR2019**)**, the co-location was typically based on matching through modelled XCO_2/XCH_4 fields and results of the comparison reported here can be expected to show larger biases and standard deviations.

Temporal

Matching SRFP soundings with TCCON sites for time is a comparatively simple operation, selecting only those TCCON values whose observation time falls within ±2 hours of each GOSAT-2 sounding time. The average is taken of all TCCON points fitting the above criteria for each SRFP sounding to provide the TCCON value against which to compare.

4 Error results

In this section we report on the comparison of the GOSAT-2 SRFP XCH4 data versus co-located GOSAT-1 and TCCON measurements as well as correlations of the bias between GOSAT-2 and TCCON with important retrieval and/or atmospheric parameters.

4.1 Overview GOSAT-1 statistics

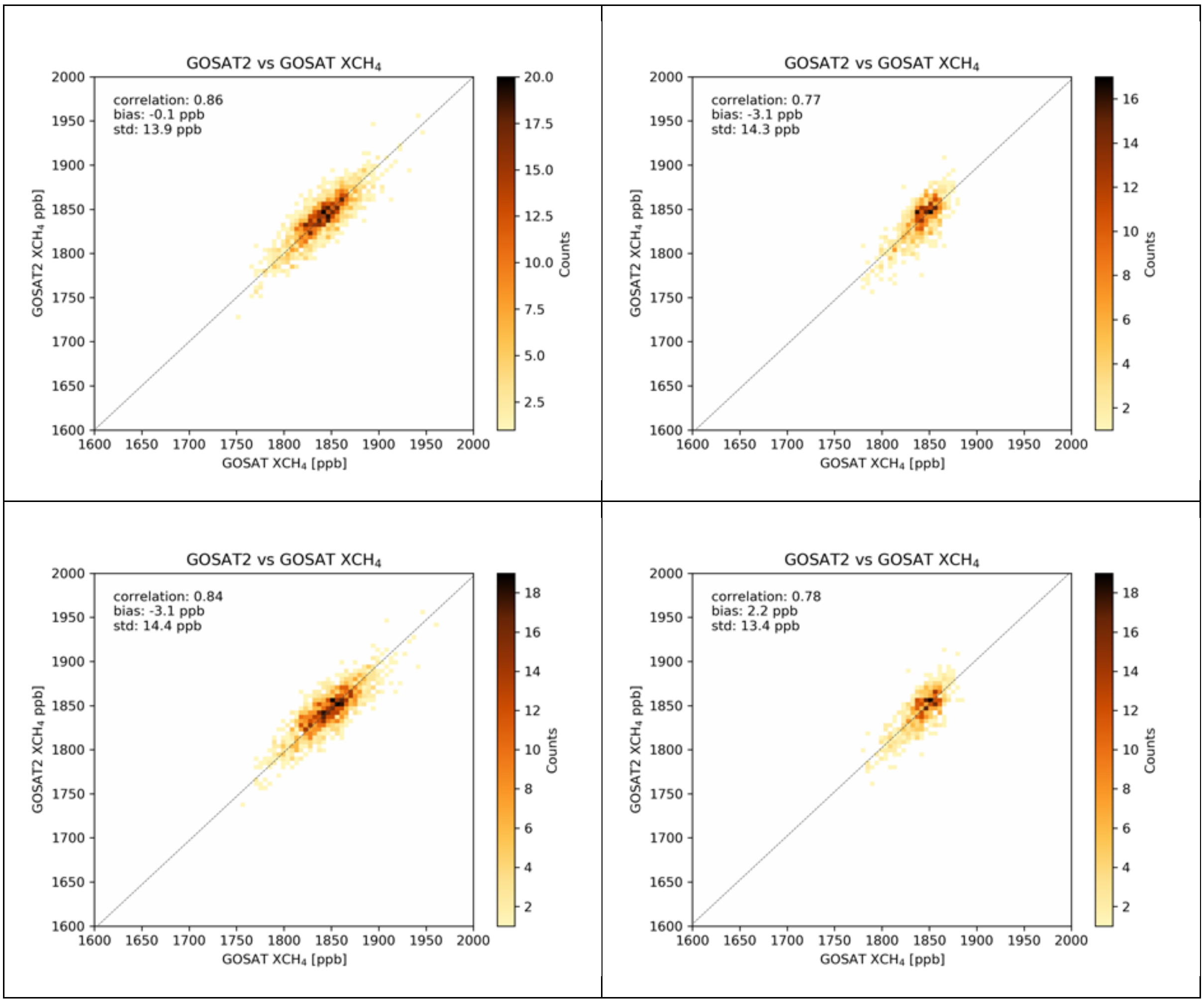


Figure 4.1: Comparison of normal (left) and glint (right) single soundings of FP-CH_4 with co-located GOSAT and GOSAT-2 measurements for the period Feb-Aug 2019. The top figures show the comparison of the non-bias corrected products and the bottom two figures the bias corrected products.

Figure 4.1 shows a comparison of GOSAT-2 and GOSAT FP-CH4 for both the non- (top) and bias-corrected (bottom) product. Table 4.1 shows a summary of the corresponding statistics.

The bias-correction of the non-glint observations has been performed with TCCON observations as described in the following section, while the glint observations have been corrected using the GOSAT-1 bias corrected product. Overall the products compare fairly well with relatively small biases, high correlations and standard deviations smaller than those found in the comparison with TCCON. The land based "bias-corrected" comparison shows a worse bias and standard deviation than the non-corrected version. This is potentially due to the small number of TCCON sites with available data for 2019, creating a non-representative correction for GOSAT-1 to GOSAT-2 co-locations away from the TCCON locations.

Table 4.1. Summary of the comparison of FP-CH4 GOSAT vs GOSAT-2 for daily 2°x2° mean concentrations. Period covered is Feb 2019 to Aug 2019.

Land	N	R	µ	σ	Glint	N	R	µ	σ
Non-corrected	1397	0.86	-0.1	13.9	Non-corrected	676	0.77	-3.1	14.3
Bias-corrected	1397	0.84	-3.1	14.4	Bias-corrected	676	0.78	2.2	13.4

4.2 Overview statistics

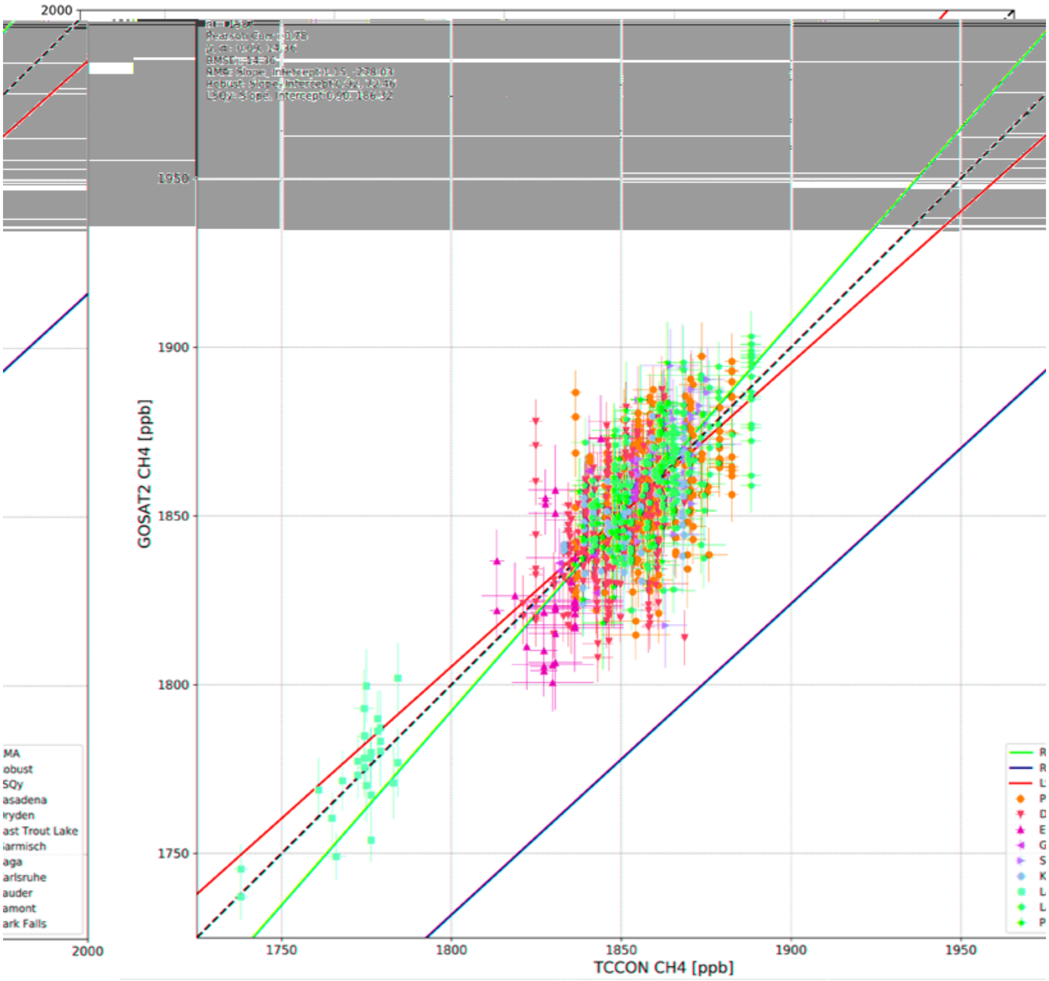


Figure 4.2: Validation of non-glint single soundings of FP-CH_4 with co-located TCCON measurements at all TCCON sites for the period Feb-Oct 2019. Numbers in the figures: μ = bias, i.e., average of the difference; σ = single measurement precision, i.e., standard deviation of the difference; N = number of co-locations.

The above figures all show a strong correlation of the retrieved (bias-corrected) XCH4 with the TCCON XCH4 (r ~ 0.78). This gives us confidence that our bias correction based on the retrieved albedo works correctly and takes out most of the bias.

The tables below (4.2 & 4.3) show in detail for each station the remaining bias and standard deviation for the co-located GOSAT-2 soundings. The time-series for the sites are shown in Figure 4.3. Mind that the values are averages per overpass for both the TCCON (blue) and GOSAT-2 (red) observations, and all values are shown, not just the co-located averages.

The spatial accuracy (standard deviation site biases) is 2.4 ppb. The most notable outliers are Garmisch, with a remaining bias of 4.18 and East Trout Lake on the other end of the spectrum with a remaining bias of -3.63 ppb. The origin for this large difference is potentially due to the low number of co-locations in combination with a few outlier values as can be seen in Figure 4.3.

Table 4.2: Overview of the SRFP/RemoTeC XCH_4 validation with TCCON (after bias correction).

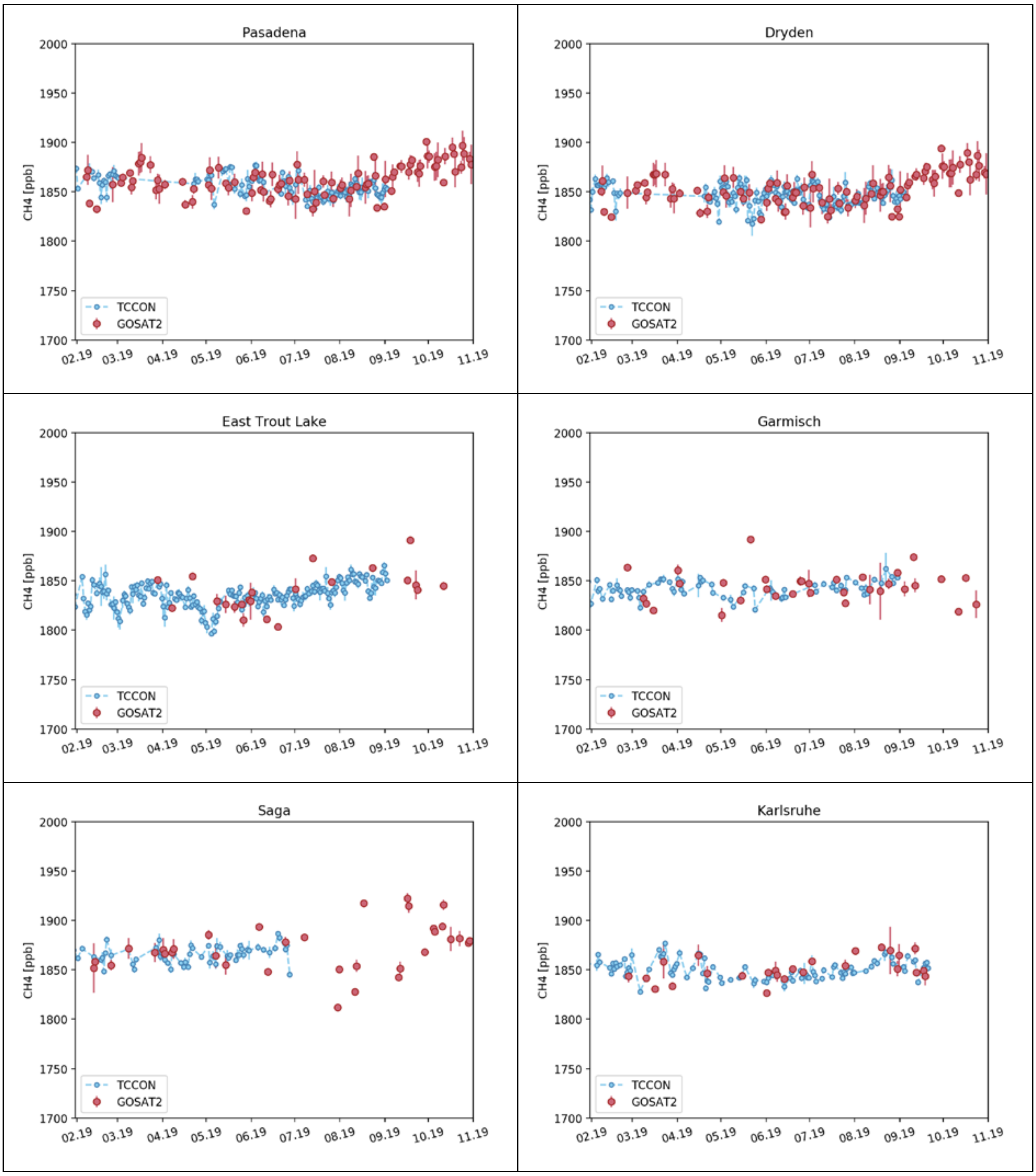
TCCON site	Number of co-locations [-]	Mean difference [ppb]	Standard deviation of difference [ppb]
Pasadena, USA	337	-2.03	15.70
Dryden, USA	448	0.22	15.36
East Trout Lake, Canada	62	-3.63	17.31
Garmisch, Germany	28	4.18	8.41
Saga, Japan	98	2.18	12.53
Karlsruhe, Germany	115	-1.31	11.17
Lauder, New Zealand	52	2.63	10.41
Lamont, USA	344	1.12	13.18
Park Falls, USA	103	2.43	13.24
All observations	1587	0.09	14.36

As shown in Table 4.3 GOSAT-2 shows very similar results to those found for GOSAT-1 over the same period as well as the longer 2009-2019 interval. The station to station standard deviation and scatter however are somewhat larger, which is potentially due to the smaller number of sites and the relatively short interval used for the bias correction.

Table 4.3: Overview of the GOSAT-1 and GOSAT-2 FP-CH4 products vs TCCON co-located measurements. GOSAT-1 has been compared for both the Feb-2019 – August 2019 interval and the complete 2009-2019 series. The mean bias μ and single measurement precision σ are calculated by taking the mean and standard deviation of the differences of all GOSAT-2 and TCCON pairs.The mean of the site means $\bar{\mu}$ and the spatial accuracy $\sigma_{\bar{\mu}}$ are calculated by taking the mean and standard deviation of the site means. The mean standard deviation $\bar{\sigma}$ and and standard deviation of the standard deviations $\sigma_{\bar{\sigma}}$ are calculated by taking the mean and the standard deviation of the site standard deviations. All units except the number of observations N, are in ppb.

Land	FP				
Variable	N	μ	σ	$\bar{\mu} \pm \sigma_{\bar{\mu}}$	$\bar{\sigma} \pm \sigma_{\bar{\sigma}}$
GOSAT2	1587	0.1	14.4	0.6±2.4	13.0±2.6
GOSAT1	964	6.13	14.4	4.8±4.6	11.8±1.9
GOSAT1 (2009-2019)*	8831	1.5	12.7	1.6±2.3	12.5±1.5

***12 stations were used for the 2009-2019 comparison, including Bialystok, Bremen, Darwin, Garmisch, Saga, Karlsruhe, Lauder, Lamont, Orleans, Park Falls, Sodankyla, and Wollongong.**



Pasadena
Dryden
East Trout Lake
Garmisch
Saga
Karlsruhe
CH4 [ppb]
2000
1950
1900
1850
1800
1750
1700
02.19
03.19
04.19
05.19
06.19
07.19
08.19
09.19
10.19
11.19
TCCON
GOSAT2

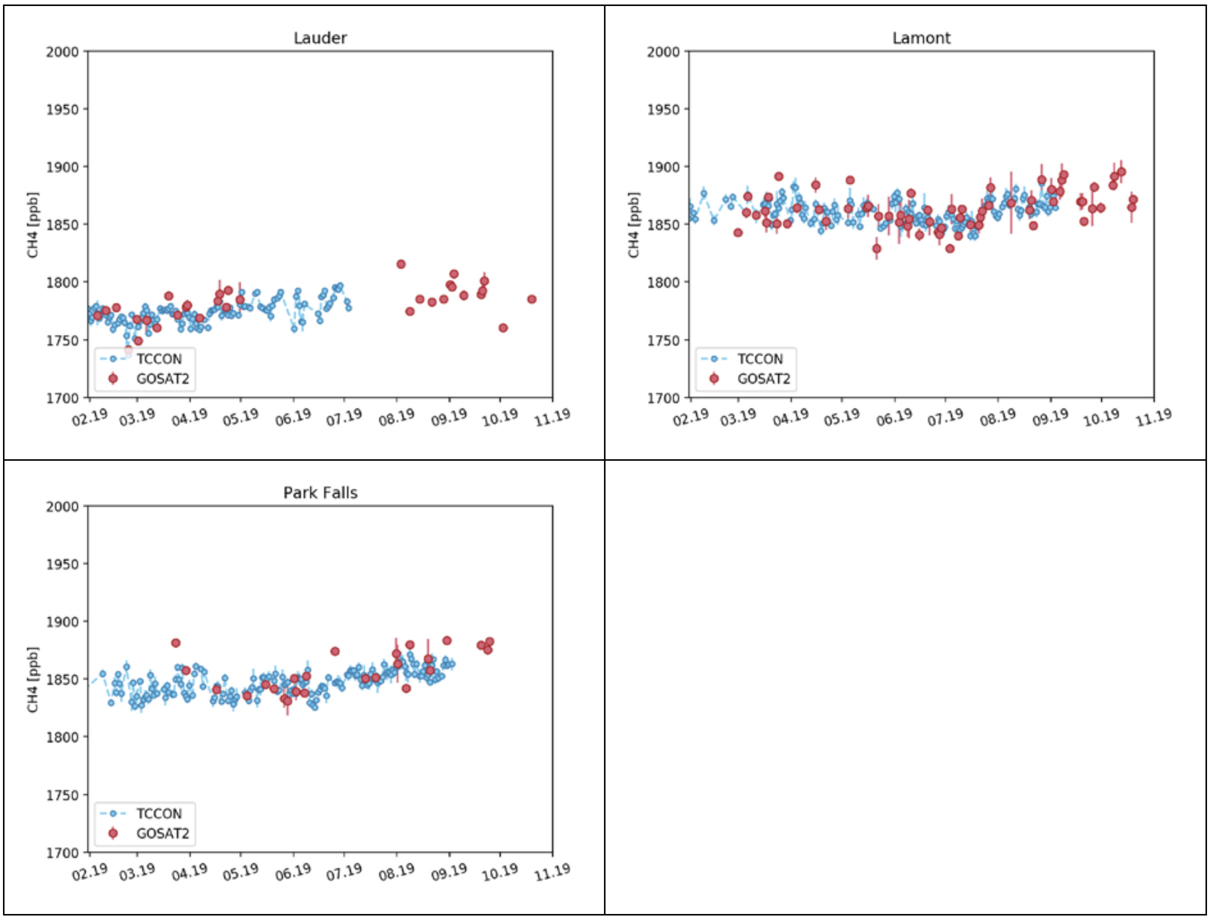


Figure 4.3 Comparison of non-glint single soundings of FP-CH_4 (red) with co-located TCCON (blue) measurements at all TCCON sites for the period Feb-Oct 2019.

4.3 Stability

As only nine months of data are available, and most FTIR sites only updated until mid-2019 we did not investigate the variations of the bias between TCCON and GOSAT-2 XCH4. Such a comparison will be added future updates of this report.

4.4 Correlations

In this section we investigate the correlation of the observed difference between TCCON and GOSAT-2 (after bias correction) with secondary retrieval or input parameters.

All correlations shown are after we performed a bias correction, which is the following:

$$\mathrm{XCH4}_{\mathrm{corr}} = \mathrm{XCH4} * (a + b * \alpha)$$

For non-sunglint observations, with a = 0.9957, b = 0.0251, and α = albedo at 1.6 µm in band 2, and,

$$\mathrm{XCH4}_{\mathrm{corr}} = \mathrm{XCH4} * (a + b * \mathrm{RO2})$$

For sunglint observations with a = 1.4208, b = 0.4254, and RO2 the retrieved O2 ratio. After applying the above bias correction for the non-sunglint observations, the remaining correlations are not very strong.

Our philosophy is however to keep the bias correction as simple as possible using a physical retrieved parameter that can explain / correct for most of the observed bias. In our case that is the retrieved albedo in band 2.

4.5 Sunglint

The GOSAT-2 bias correction for sunglint observations has been based on the GOSAT-1 bias corrected product, and the choice of parameters have been kept the same as used in the GOSAT-1 correction. When the TCCON datasets are updated, we will update the bias correction of the sunglint and this section of the manuscript.

4.6 Random error

The error that comes out of the RemoTeC retrieval is just a purely statistical error on the radiance that has been propagated through the entire retrieval chain.

In order to more accurately estimate the actual random error on the GOSAT-2 sounding, we applied the following procedure to obtain a scaling factor to scale our statistical error. We take the absolute difference of every co-located sounding and divide it by the retrieved statistical error corresponding to that sounding. We then average these values to obtain the average scaling factor by which to scale the retrieved statistical error to obtain a more correct estimate of the random error.

Based on the analysis, we obtain the following scaling factors for the SRFP XCH4 product,1.44 for normal mode and 1.38 for sunglint mode. Subsequently, we calculate the uncertainty ratio which is defined as the ratio of the mean value of the reported uncertainty and the standard deviation of the difference to TCCON. We obtain uncertainty ratios of 0.69 for normal mode and 0.72 for sunglint mode.

The uncertainties in the product are already scaled and represented by the parameter "xch4_uncertainty". The unscaled values are added under the parameter name "raw_xch4_err".

5 Conclusions

This report summarizes the performance of the RemoTeC GOSAT-2 SRFP XCH4 retrieval. In general, we find very good agreement with GOSAT-1 and TCCON data. All comparisons show a high degree of correlation and show biases and standard deviations of that are very similar to the GOSAT-1 SRFP product.

The spatial accuracy (standard deviation site biases) is 2.4 ppb and a single measurement precision of around 14.36 ppb is observed. Correlations of the observed bias with retrieved parameters were also checked and it was found that after the initial bias correction based on the retrieved albedo in Band 2 the remaining correlations with other parameters were very small and not significant.

6 References

/ATBD 2020/ T. Krisna and the GHG-CCI group at SRON: ESA Climate Change Initiative "Plus" (CCI+) ATBD (ATBDv1.1) for the RemoTeC CH4 GOSAT-2 Data Product CH4_GO2_SRFP for the Essential Climate Variable (ECV) Greenhouse Gases (GHG), ESA GHG CCI+, 2020.

/Buchwitz et al., 2013/ Buchwitz, M., M. Reuter, O. Schneising, H. Boesch, S. Guerlet, B. Dils, I. Aben, R. Armante, P. Bergamaschi, T. Blumenstock, H. Bovensmann, D. Brunner, B. Buchmann, J. P. Burrows, A. Butz, A. Chédin, F. Chevallier, C. D. Crevoisier, N. M. Deutscher, C. Frankenberg, F. Hase, O. P. Hasekamp, J. Heymann, T. Kaminski, A. Laeng, G. Lichtenberg, M. De Mazière, S. Noël, J. Notholt, J. Orphal, C. Popp, R. Parker, M. Scholze, R. Sussmann, G. P. Stiller, T. Warneke, C. Zehner, A. Bril, D. Crisp, D. W. T. Griffith, A. Kuze, C. O'Dell, S. Oshchepkov, V. Sherlock, H. Suto, P. Wennberg, D. Wunch, T. Yokota, Y. Yoshida, The Greenhouse Gas Climate Change Initiative (GHG-CCI): comparison and quality assessment of near-surface-sensitive satellite-derived CO2 and CH4 global data sets, Remote Sensing of Environment, doi:10.1016/j.rse.2013.04.024, in press (http://authors.elsevier.com/sd/article/S0034425713003520), 2013.

/Butz et al., 2011/ Butz, A., et al.: Toward accurate CO2 and CH4 observations from GOSAT Geophys. Res. Lett., 38(L14812), doi:10.1029/2011GL047888, 2011

/Butz et al., 2009/ Butz, A., O. P. Hasekamp, C. Frankenberg, and I. Aben: Retrievals of atmospheric CO2 from simulated space-borne measurements of backscattered near-infrared sunlight: accounting for aerosol effects Appl. Opt.,48(18), 3322–3322–, 2009

/Butz et al., 2010/ Butz, A., O. P. Hasekamp, C. Frankenberg, J. Vidot, and I. Aben, CH4 retrievals from spacebased solar backscatter measurements: performance evaluation against simulated aerosol and cirrus loaded scenes, J. Geophys. Res., 115, D24302, doi:10.1029/2010JD014514, 2010

/CECR2017/ R. Detmers, Comprehensive Error Characterisation Report : SRON full-physics retrieval algorithm for XCH4 (SRFP-XCH4) for the Essential Climate Variable (ECV) Greenhouse Gases (GHG) 2017.

/C3SPQAR2019/ L. Wu**,** Product Quality Assessment Report (PQAR) – ANNEX B for products CO2_GOS_SRFP (v2.3.8, 2009-2018) & CH4_GOS_SRFP (v2.3.8, 2009-2018) C3S_312a_Lot6_IUP-UB – Greenhouse Gases, 2019.

/Chevalier et al., 2014/ Chevalier, F., Palmer, P.I., Feng, L., Boesch, H., O'Dell, C.W., Bousquet, P., Towards robust and consistent regional CO2 flux estimates from in situ and space-borne measurements of atmospheric CO2, Geophys. Res. Lett., 41, 1065-1070, DOI:10.1002/2013GL058772, 2014

/Schepers et al., 2012/ Schepers, D., S. Guerlet, A. Butz, J. Landgraf, C. Frankenberg, O. Hasekamp, J.-F. Blavier, N. M. Deutscher, D. W. T. Griffith, F. Hase, E. Kyro, I. Morino, V.

Sherlock, R. Sussmann, I. Aben, Methane retrievals from Greenhouse Gases Observing Satellite (GOSAT) shortwave infrared measurements: Performance comparison of proxy and physics retrieval algorithms, J. Geophys. Res., 117, D10307, doi:10.1029/2012JD017549, 2012.

/Wagner et al., 2012/ Wagner, W., Dorigo, W., de Jeu, R., Parinussa, R., Scarrott, R., Kimmo, Lahoz, W., Doubková, M., Dwyer, N. and Barrett, B.: ESA Soil Moisture CCI: Comprehensive Error Characterisation Report. [online] Available from: http://www.esa-soilmoisture-cci.org/sites/default/files/documents/public/Deliverables%20-%20CCI%20SM%201/20120521_CCI_Soil_Moisture_D1.2.1_CECR_v.0.7.pdf (Accessed 25 January 2016), 2012.

/Wunch et al., 2015/ Wunch, D., Toon, G.C., Sherlock, V., Deutscher, N.M., Liu, X., Feist, D.G., Wennberg, P.O., The Total Carbon Column Observing Network's GGG2014 Data Version. Carbon Dioxide Information Analysis Center, Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA (available at: doi:10.14291/tccon.ggg2014.documentation.R0/1221662), 2015.