ESA Climate Change Initiative “Plus” (CCI+)

End-to-End ECV Uncertainty Budget (E3UB) Version 5.0

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For the RemoTeC XCH4 GOSAT-2 SRON Proxy Product

(CH4_GO2_SRPR) Version 2.0.3

for the Essential Climate Variable (ECV)

Greenhouse Gases (GHG)

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Change log

Version Nr.	Date	Status	Reason for change
Version 1.0	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
Version 4.0	18. Apr. 2023	As submitted	- Updated doc to version 4.0 - Quality filtering via random forest model prediction
Version 5.0	11. July 2024	As submitted	- Update doc to version 5.0 - New product version v2.0.3 - Timeseries extended to end of 2023

Table of Contents

Executive summary

This report summarizes the performance of the RemoTeC GOSAT-2 SRPR XCH_4 retrieval. In general, we find very good agreement with TCCON and GOSAT data for the two modes (land and ocean). The mean bias (global offset) is -0.23 ppb with a single measurement precision of 15.69 ppb. The spatial accuracy (standard deviation site biases) is 5.2 ppb. Based on comparison with TCCON we scale the retrieved statistical error by a factor 1.84 for land mode and 1.58 for glint mode to obtain a representative random error. This corresponds to an uncertainty ratio of 0.81 for land mode and 0.77 glint mode.

Estimates of achieved data quality:					
Product ID	**Algorithm**	**Single measurement precision (1-sigma) in [ppb]**	**Mean bias (global offset) [ppb]**	**Spatial Accuracy: Relative systematic error [ppb]**	**Uncertainty ratio (scaling)**
CH4_GO2_SRPR	RemoTeC	15.69	-0.23	5.2	0.81

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

1 Introduction

1.1 Purpose of document

This E3UB provides an overview of random and systematic errors affecting the SRON Proxy XCH_4 retrieval submitted for the ESA GHG-CCI+ Climate Research Data Package 9. 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 Proxy XCH_4 product for flux 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.
Sensitivity	Change of measurement due to instrumental and algorithmic response to physical or simulated input parameters.

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 (e.g. 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 receives 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 SRPR

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 (Butz et al., 2009; Butz et al., 2010; Butz et al., 2011, Schepers et al 2012) which is also used used for the GOSAT retrievals. 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. A small difference between the GOSAT and -2 retrievals is that the GOSAT-2 retrieval uses a slightly shortened retrieval window for the O_2-A Band as described in the version 1.0 ATBD document **(**Krisna et al. 2020**)**. 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). The inversion products used for XCO_2 are the official CAMS products (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 GGG2020 release of the TCCON data. The CH4_GO2_SRPR product v2.0.3 covers the period from start of measurements (February 2019) up until the end of December 2023. More details on the technical aspects of the retrievals can be found in the version 4.0 ATBD GO2-SRPR document (Barr et al. 2023).

3.2 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, Laughner et al. 2021). 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 GGG2020 collection (available from https://tccondata.org/).

3.2.1 Colocation

To assess the quality of GOSAT-2 Proxy product, XCH_4 observations against rigorously validated ground based TCCON values, GOSAT-2 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.

Temporal

Matching SRPR 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 SRPR sounding to provide the TCCON value against which to compare.

3.2.2 Bias Correction

From comparison with TCCON it was found that the error in XCH_4 correlates with the retrieved albedo α at 1.6 µm in band 2. Based on this correlation the following bias correction has been developed for XCH_4:

$$XCH4_{corr} = XCH4 * (a + b * \alpha) \quad (1)$$

Where we use here a = 0.9906 , b = 0.00934 for retrievals over land.

For retrievals over ocean, GOSAT-2 measures in sun-glint mode. Sun-glint mode takes advantage of specific viewing angle where the radiance of back-scattered sunlight is higher due to reflection from waves. This amplifies the albedo, allowing retrievals over ocean to be carried out, where the albedo is generally too low to retrieve accurate concentrations. We find that the error in XCH_4 correlates with the bias better for the retrieved ratio of O_2. As such we apply a similar bias correction as in equation 1 but with the O_2 ratio, r:

$$XCH4_{corr} = XCH4 * (a + b * r) \quad (2)$$

Where we take a = 0.9700 and b = 0.0215.

Following Noel et al. 2022, we parameterize the bias of GOSAT-2 and TCCON through:

$$\Delta X = a_0 + a_1 t + a_2 \sin(2\pi t + a_3) + \varepsilon \quad (3)$$

Where equation 3 is fit to the bias of colocated data from each station individually. a_0 is a constant bias term, a_1 represents a linear term, a_2 measures the amplitude of the seasonal variation of the bias, and a_3 measures the temporal shift of the seasonal term, and ε is an error term. TCCON sites are considered only if there are more than 50 colocations.

We then define Δ_{reg} as the regional bias and defined as the mean of ΔX from equation 3 and Δ_{seas} is the seasonal bias, defined as the standard deviation of the seasonal (sine) term in equation 3. Δ_{spt} is the spatio-temporal component of the bias, defined as Δ_{reg} and Δseas added in quadrature. Finally Δ_{dri} is the linear drift, and calculated as a_1 from equation 3. We further define the station-to-station bias, δ, as the standard deviation of the individual site biases.

3.3 Satellite Inter-comparison

The GOSAT Proxy XCH4 product (SRPR) has been extensively validated and offers an excellent opportunity for comparison. 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 is discarded.

4 Error results

In this section we report on the comparison of the GOSAT-2 Proxy XCH_4 data providing validation of the data product using TCCON measurements and also colocations with GOSAT, for retrievals over both land and ocean.

4.1 Overview TCCON statistics

Figures 4.1 and 4.2 show strong correlations of the retrieved (bias-corrected) XCH_4 with the TCCON XCH_4 (r ~ 0.9). This gives us confidence that our bias correction based on the retrieved albedo works correctly and takes out most of the bias.

Tables 4.2 and 4.3 show in detail for each station the remaining bias and standard deviation for the co-located GOSAT-2 soundings. We emphasise that the parameters for glint mode are derived only from a few stations due the low number of data points. Table 4.3 summarises the statistics of the TCCON validation.

The time-series for the sites are shown in Figures 4.3 and 4.4. Daily averages of XCH_4 are provided for TCCON as the variation throughout the course of one day are minimal at TCCON stations, whereas all collocated GOSAT-2 measurements are provided.

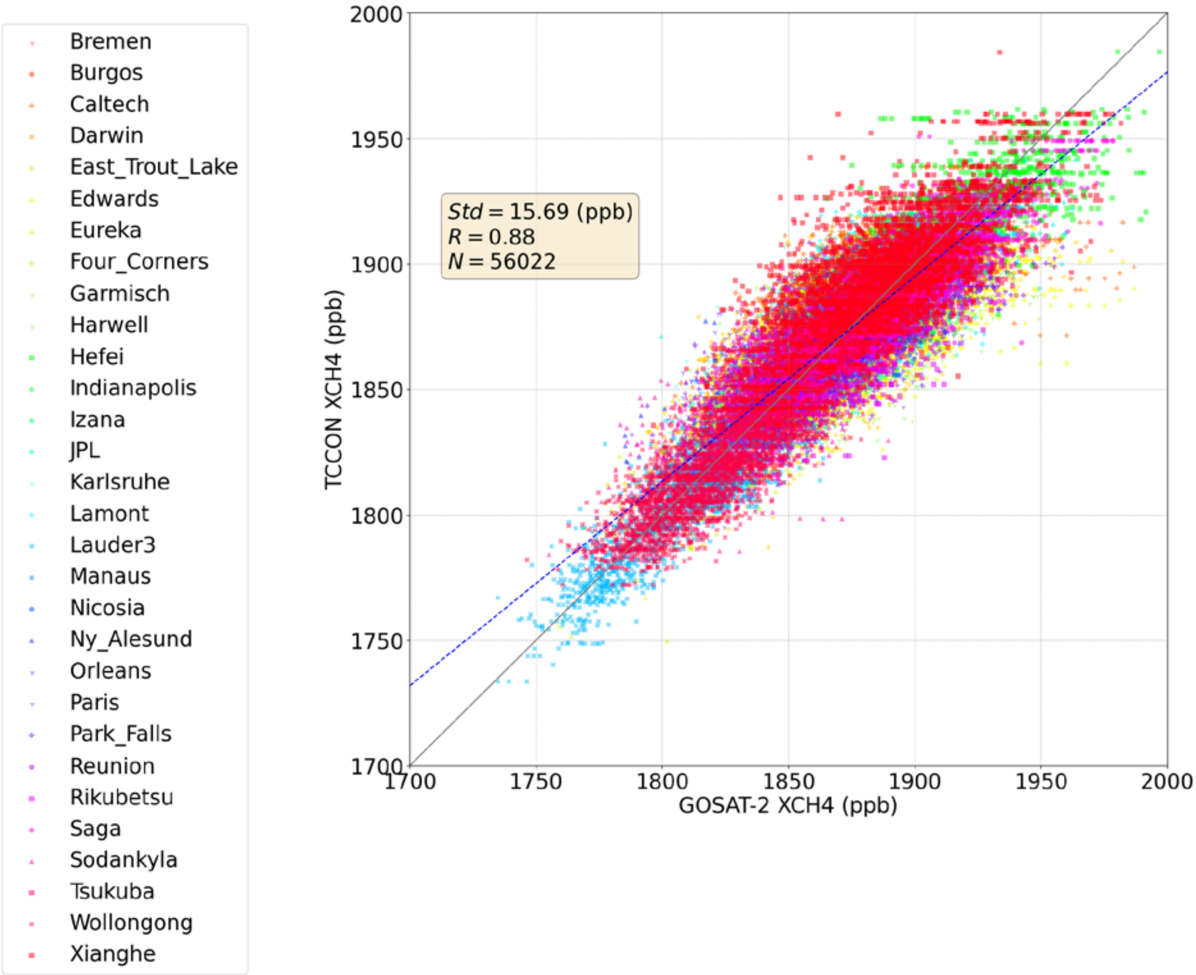

Figure 4.1 GOSAT-2 XCH_4 for soundings over land plotted against TCCON, for the RemoTeC Proxy product. Data are compared only if they are fully colocated in space and time. The standard deviation of the population, Pearson's correlation coefficient and number of retrievals are given in the inset. The legend plots the different TCCON stations where markers are as follows. Stations that are along the coast and also sensitive to glint mode (ocean) measurements are indicated as circles. Those that have high latitudes in the northern and southern hemispheres are upward triangles and crosses, respectively. Stations in Asia, North America and Europe are indicated by squares, pluses and downward triangles respectively.

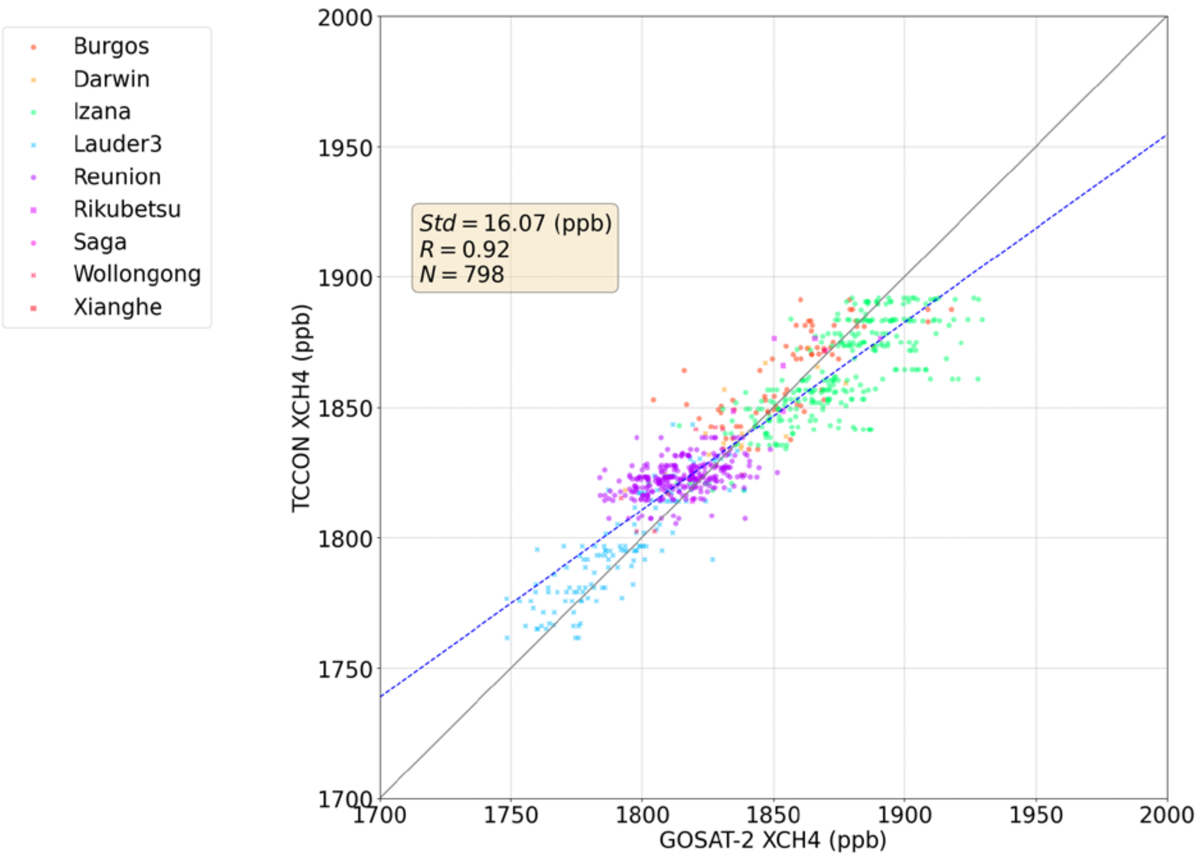

Figure 4.2 Same as Figure 4.1 but for soundings taken in glint mode.

Table 4.1: Overview of TCCON validation of XCH_4 from the GOSAT-2 Proxy product

TCCON site [Land mode]	Δreg (ppb)	Δseas (ppb)	Δdri (ppb yr^{-1})	Δspt (ppb)	N
Bremen	-0.29	5.94	5.6	5.95	276
Burgos	3.53	1.54	-1.51	3.85	535
Caltech	-6.96	0.66	1.24	6.99	9551
Darwin	-2.62	3.0	1.8	3.99	1073
East Trout Lake	0.19	1.94	-0.65	1.95	2991
Edwards	5.82	3.55	-1.26	6.82	10642
Eureka	-4.42	6.7	0.65	8.02	165
Garmisch	9.61	1.8	0.14	9.78	1523
Harwell	0.55	3.39	-1.5	3.43	1239
Hefei	2.51	3.0	0.73	3.91	1183
Karlsruhe	-1.46	4.3	0.66	4.54	1500
Lamont	0.99	5.42	-3.5	5.51	3910
Lauder3	2.82	1.79	-0.17	3.34	2163
Nicosia	1.53	1.31	3.86	2.02	864
Ny Alesund	-16.0	6.75	1.63	17.37	115
Orleans	-1.48	5.3	6.96	5.5	1268
Paris	-0.17	5.49	5.62	5.49	1322
Park Falls	2.72	2.93	-1.83	4.0	2573
Rikubetsu	7.75	2.08	0.71	8.02	858
Saga	2.63	0.6	0.86	2.7	3065
Sodankyla	-2.08	5.63	-2.2	6.0	1527
Tsukuba	-3.38	4.14	5.54	5.34	798
Wollongong	0.87	1.62	0.25	1.84	3032
Xianghe	-8.26	1.88	4.89	8.47	3813

Table 4.2: Overview of the Proxy XCH_4 validation with TCCON (after bias correction) for ocean retrievals.

TCCON site [Land mode]	Δreg (ppm)	Δseas (ppm)	Δdri (ppm yr^{-1})	Δspt (ppm)	N
Burgos	2.28	5.23	1.36	5.7	70
Izana	13.85	7.02	-1.79	15.53	289
Lauder3	-9,24	7.14	-4.33	11.67	130
Reunion	-6.24	0.38	11.86	6.25	277

Table 4.3: Overview of the GOSAT-2 XCH_4 products vs TCCON co-located measurements. N is the number of collocated measurements, μ is the mean bias, σ is the single measurement precision, γ is the linear drift term, δ is the station-to-station bias, and R is the correlation coefficient.

	Proxy					
Variable	N	μ (ppb)	σ (ppb)	γ (ppb yr^{-1})	δ (ppb)	R
GOSAT2 Land	56022	-0.23	15.69	1.18	5.2	0.88
GOSAT-2 Ocean	798	0.16	16.07	1.77	9.0	0.92

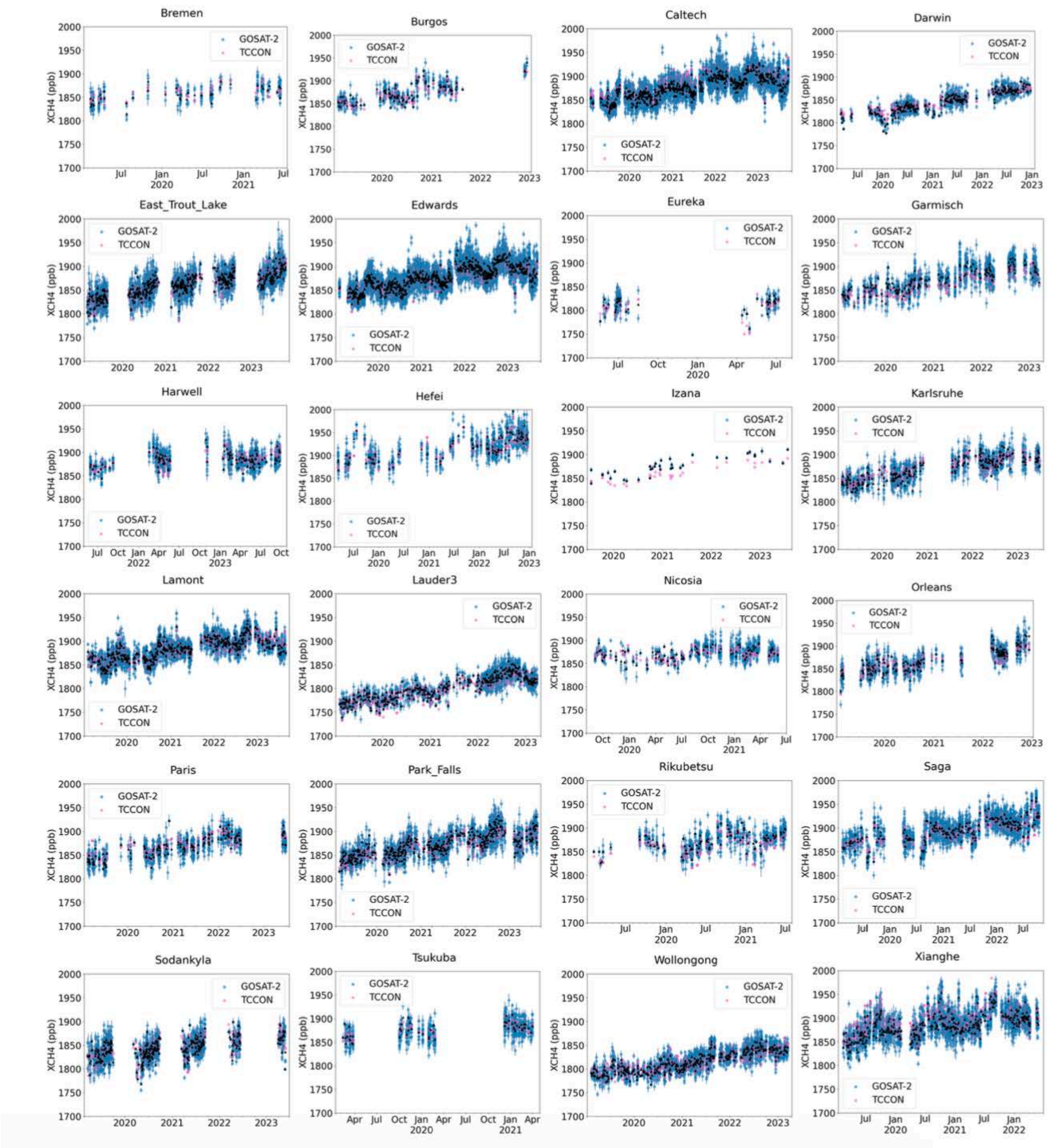

Figure 4.3 Comparison of land single soundings of XCH_4 from the Proxy retrieval (blue circles) with co-located TCCON (pink triangles) measurements at all TCCON sites.

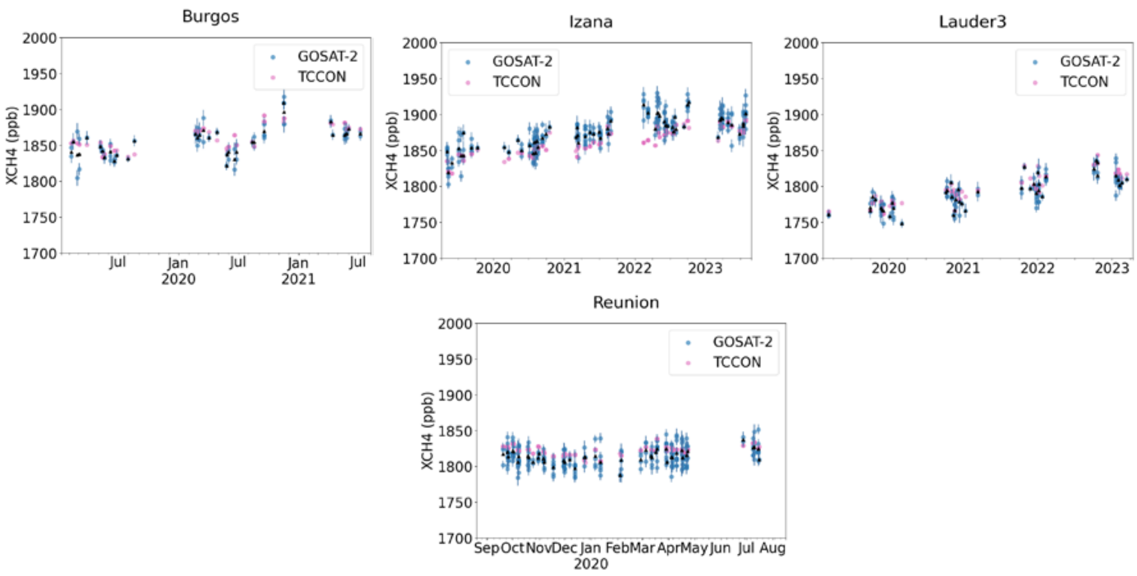

Figure 4.4 Same as Figure 4.3 but for soundings taken in glint mode.

4.2 GOSAT-2 Inter-comparison with GOSAT and TROPOMI

In Figure 4.5 we show a comparison of GOSAT-2 and GOSAT XCH_4 for the bias corrected product, over 2019 to 2023. The bias-correction of both observations has been performed with TCCON data as described in section 3.2.2. Overall the products compare well with relatively small biases, high correlations and standard deviations similar to those found in the comparison with TCCON.

We find a very high correlation between GOSAT and GOSAT-2 for the Proxy XCH_4 product of 0.92, higher than that of GOSAT-2 with TCCON. The bias between GOSAT and GOSAT-2 is -6.5 ppb and the standard deviation of the colocations is 13.1 ppb.

XCH_4 from TROPOMI can also be used to inter-compare with the GOSAT-2 Proxy XCH_4 product, which we also present in Figure 4.5. Here we inter-compare our GOSAT-2 product against the TROPOMI operational product, and evaluate the performance of the quality filtering on global scales. The TROPOMI product was pre-filtered with VIIRS cloud fraction using the strictest filter of < 0.001, and quality filtered using nominal quality flags. We limit the analysis to retrievals over land only.

We find a global average of the bias of only -1.4 ppb, and a standard deviation of 23.8 ppb, roughly around 1 % of XCH_4. The lower bias suggests that GOSAT-2 is in better agreement with TROPOMI than with GOSAT, however the scatter and correlation are lower for GOSAT.

4.3 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 with which 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 SRPR XCH_4 product, 1.84 for land mode and 1.58 for glint 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 0.81 for land mode and 0.77 for glint 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".

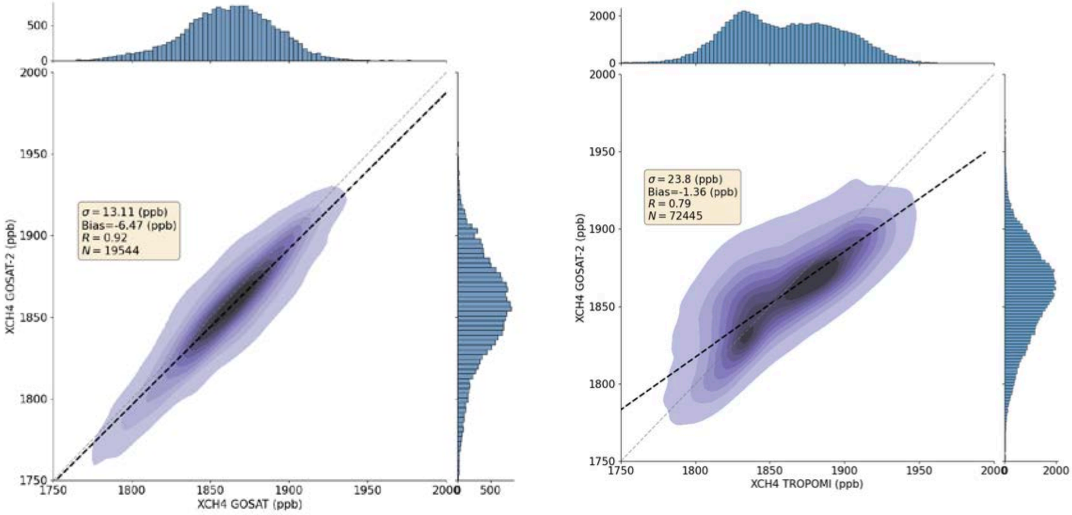

Figure 4.5. *right:* Correlation between XCH_4 measured by TROPOMI and GOSAT-2 shown as a kernel density estimation (KDE) plot. The mean bias, standard deviation, number of points and correlation coefficient of the population are also quoted. Histograms of the number of counts are shown around the margin, along with the linear regression and the 1-to-1 lines in black and grey respectively. *Left*: Same as the right but for GOSAT compared to GOSAT-2.

5 Conclusions

This report summarizes the performance of the RemoTeC GOSAT-2 Proxy data products. In general, we find very good agreement with GOSAT-2 and TCCON data. All comparisons show a high degree of correlation (r~0.9) and show biases and standard deviations of that are very similar to those found comparing GOSAT-2 and GOSAT.

From XCH_4, TCCON validation results in a single measurement precision of 15.7 ppb, station-to-station bias of 5.2 ppb and linear drift of 1.18 ppb yr^{-1}. Through intercomparison with GOSAT, we find a bias of -6.5 ppb between GOSAT and GOSAT-2. The standard deviation is 13.1 ppb and correlation coefficient is 0.92. The global average bias of GOSAT-2 with TROPOMI is less (only -1.4 ppb) however the standard deviation is a factor of 2 higher compared to the GOSAT-GOSAT2 inter-comparison, and the correlation also lower, but still high (0.79).

The statistical error is scaled by a factor of 1.84 and 1.58 for land and ocean retrievals respectively, to obtain a representative random error. We find a corresponding uncertainty ratio of 0.81 for land, and 0.77 for ocean, measurements.

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