ESA Climate Change Initiative "Plus" (CCI+)

End-to-End ECV Uncertainty Budget (E3UB) Version 4.0

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For the RemoTeC XCO2 GOSAT-2 SRON Full-Physics Product (CO2_GO2_SRFP) Version 2.0.2

for the Essential Climate Variable (ECV)

Greenhouse Gases (GHG)

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Change log

Version Nr.	Date	Status	Reason for change
Version 1	27. Oct. 2020	Draft	New document
Version 1.1	04. Jan. 2021	As submitted	- Definition uncertainty ratio - Update format - Remove typos
Version 1.1	04. Feb. 2021	As submitted	- Update after ESA reviews - Remove typos
Version 2.0	04. Nov. 2021	As submitted	- Update L2 processing: Filter criteria, selection of TCCON station, and bias correction - Update comparison with GOSAT
Version 3.0	27. Jan. 2022	As submitted	- Update doc to version 3.0
Version 4.0	18. Apr. 2023	As submitted	- Update doc to version 4.0 - Quality filtering via random forest model prediction

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Executive summary

This report summarizes the performance of the RemoTeC GOSAT-2 SRFP XCO_2 retrieval. In general, we find very good agreements with respect to TCCON data for the two modes, land and ocean (sun-glint), with high correlations. The mean bias (so-called global offset) is -0.01 ppm with a single measurement precision of 2.21 ppm. The spatial accuracy (so-called standard deviation site biases or station-to-station variability) is 0.5 ppm and mean standard deviation of around 2.3 ppm is observed for most TCCON stations.

Based on comparison with TCCON, we scale the retrieved statistical error by a factor of 2.36 and 3.24 for land and ocean retrievals respectively, to obtain a representative random error. Using this approach, we find a corresponding uncertainty ratio of 0.83 for land, and 0.82 for ocean, measurements.

Table 1: An overview of the achieved data quality for the XCO_2 SRFP product.

Estimates of achieved data quality: CO2_GO2_SRFP					
Sensor	**Algorithm**	**Single measurement precision (1-sigma) in [ppm]**	**Mean bias (global offset) [ppm]**	**Spatial Accuracy: Relative systematic error [ppm]**	**Uncertainty ratio (scaling)**
TANSO-FTS-2 on GOSAT-2	RemoTeC	2.21	-0.01	0.50	0.83

1 Introduction

1.1 Purpose of document

This E3UB provides an overview of random and systematic errors affecting the SRON SRFP XCO_2 retrieval submitted for the ESA GHG-CCI+ Climate Research Data Package 8. 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 XCO_2 concentration change (Buchwitz et al., 2011; 2014).

1.2 Intended audience

This document is intended for users in the modelling community applying the SRFP XCO_2 product for CO_2 inversions, as well as remote sensing experts interested in atmospheric soundings of XCO_2. 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 Retrieval Algorithm

The RemoTeC algorithm is used to simultaneously retrieve XCH_4 and XCO_2 based on the NIR and SWIR radiance spectra measured by the TANSO-FTS-2 on GOSAT-2. The algorithm was originally developed by SRON and the Karlsruhe Institute of Technology (KIT) (Butz et al., 2009; Butz et al., 2010; Butz et al., 2011; Schepers et al., 2012). For the retrieval, we analyze four spectral regions: the 0.77 µm O_2 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 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 in combination with a surface elevation data base.

The retrieved XCO_2 has been validated with respect to ground based TCCON measurements. To further improve accuracy, a bias correction has been developed based on the TCCON comparisons. For the validation and the bias correction, we use the GGG2020 release of the TCCON data (Wunch et al., 2015, Laughner et al. 2021)**.** Detailed descriptions on the technical aspects of the retrieval can be found in the ATBD GO2-SRFP document (Barr et al. 2023).

3.2 TCCON Validation

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 GGG2020 collection (available from https://tccondata.org/).

3.2.1 Co-location

To assess the quality of SRFP retrieval XCO_2 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.

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.

3.2.2 Bias Correction

From comparison with TCCON it was found that the error in XCO_2 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 XCO_2:

$$XCO2_{corr} = XCO2 * (a + b * \alpha) \tag{1}$$

Where we use here a = 0.99023 , b = 0.05021 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 XCO_2 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:

$$XCO2_{corr} = XCO2 * (a + b * r) \tag{2}$$

Where we take a = 1.46845 and b = -0.47389.

3.3 Comparison to GOSAT SRFP

The GOSAT SRPR retrieval (CO2_GOS_SRFP product) has been extensively validated and offers an excellent opportunity for comparison. We split the GOSAT-2 observations into land (ocean) 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 is discarded.

4 Error results

In this section we report on the comparison of the GOSAT-2 SRFP XCO_2 data versus co-located TCCON measurements as well as correlations of the bias between GOSAT and TCCON with important retrieval and/or atmospheric parameters.

4.1 Overview TCCON statistics

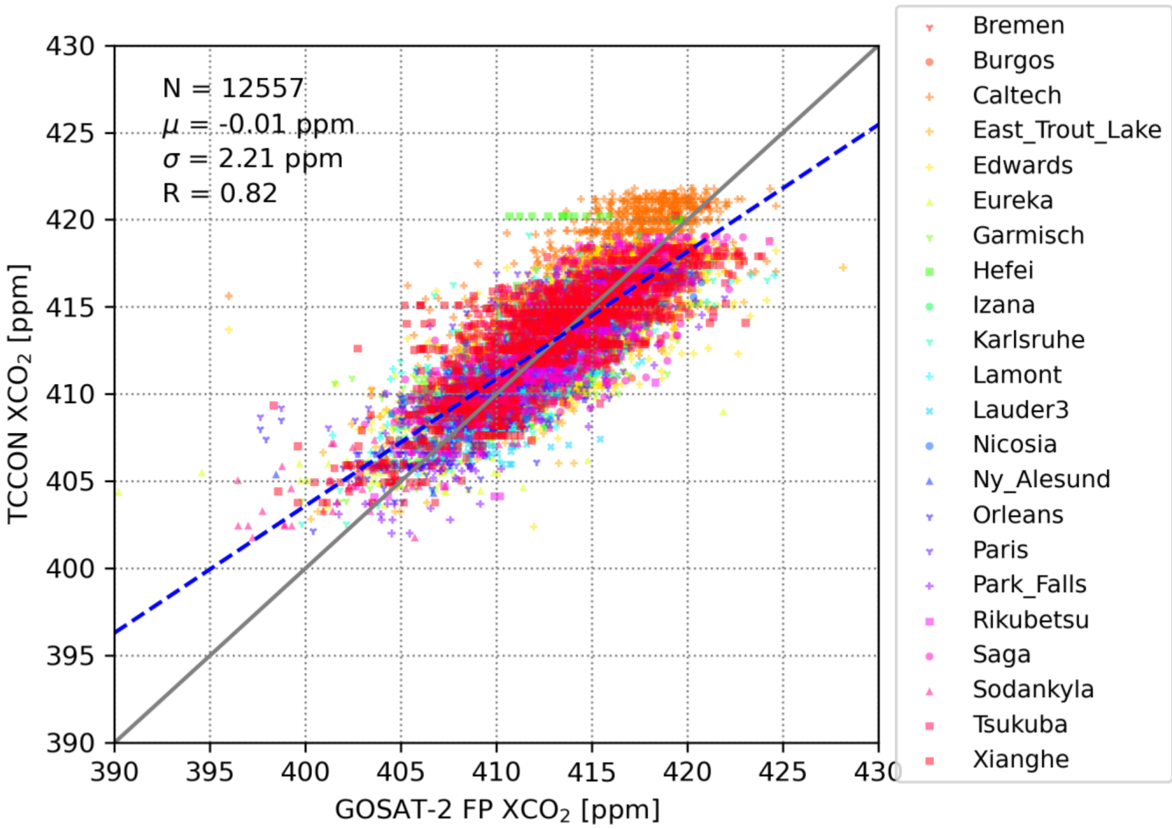

Figure 4.1: Validation of land single soundings of XCO_2 with co-located TCCON measurements at all TCCON sites for the period Feb 2019 to end Dec 2021. Numbers in the figures: μ = bias, i.e., average of the difference; σ = single measurement precision, i.e., standard deviation of the difference; N = number of co-locations; R the correlation coefficient. 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. Error bars are not shown due to the large number of data points, however they are of a similar order to those shown in Figure 4.2.

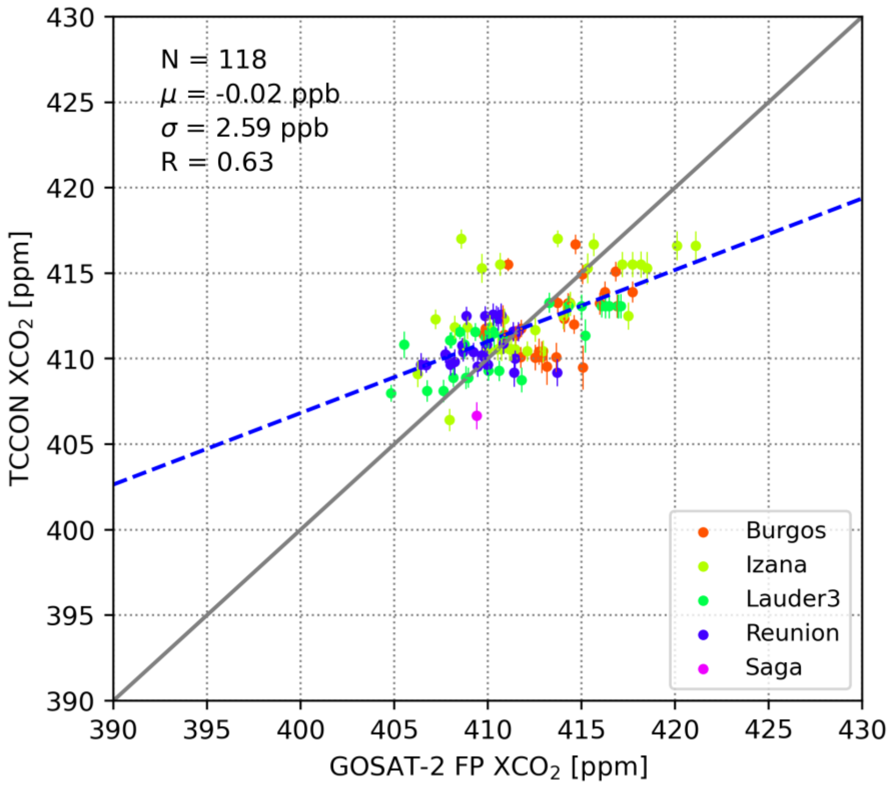

Figure 4.2 Validation of ocean single soundings of XCO_2 with co-located TCCON measurements at all TCCON sites for the period Feb 2019 to end Dec 2021. Numbers in the figures: μ = bias, i.e., average of the difference; σ = single measurement precision, i.e., standard deviation of the difference; N = number of co-locations; R the correlation coefficient. Error bars are shown on XCO_2 for GOSAT-2 as the relative error for XCH_4 from TCCON is negligible.

Figure 4.1 shows a strong correlation of the retrieved (bias-corrected) XCO_2 with the TCCON XCO_2 (r ~ 0.82). 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. The time-series for the sites are shown in Figure 4.3. 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.

The TCCON station Lauder in the Southern Hemisphere is the most notable in terms of large bias with a remaining bias after correction of 1.08 ppm. Likewise Izana has an even higher bias, of 1.73 ppm, and like Lauder is a station close to the coast, however this large bias may be a result of having only 12 colocations. Caltech also shows a large bias with -1.02 ppm and, due to the very large number of colocations at this site, influences the statistics heavily.

Ny Alesund has the lowest number of colocations with 12, and hence may not be a reliable station to include in the analysis. Excluding Ny Alesund and Izana from the validation calculations we derive a spatial accuracy of 0.5 ppm.

Table 4.2: Overview of the SRFP/RemoTeC XCO_2 validation with TCCON (after bias correction) for land retrievals .

TCCON site [Land mode]	Number of co-locations [-]	Mean difference [ppm]	Standard deviation of difference [ppm]
Bremen	139	-0.18	1.91
Burgos	129	0.40	1.97
Caltech	2580	-1.02	2.09
East_Trout_Lake	353	0.48	2.48
Edwards	3158	0.64	2.02
Eureka	89	-0.26	3.90
Garmisch	324	0.09	2.33
Hefei	136	-0.49	2.62
Izana	12	1.73	1.67
Karlsruhe	303	-0.18	2.17
Lamont	1440	0.18	1.72
Lauder	229	1.08	1.85
Nicosia	288	0.31	1.77
Ny_Alesund	8	-0.69	3.87
Orleans	303	-0.19	2.16
Paris	384	-0.15	2.26

Park_Falls	420	0.26	2.11
Rikubetsu	170	0.53	2.07
Saga	627	0.33	2.09
Sodankyla	168	-0.49	2.33
Tsukuba	349	-0.83	2.26
Xianghe	948	-0.16	2.49
All observations	12557	-0.01	2.21

Table 4.2: Overview of the SRPR/RemoTeC XCO_2 validation with TCCON (after bias correction) for ocean retrievals.

TCCON site [Glint mode]	Number of co-locations [-]	Mean difference [ppm]	Standard deviation of difference [ppm]
Burgos	26	1.21	2.25
Izana	32	-0.29	3.07
Lauder	31	0.06	2.52
Reunion	28	-1.03	1.74
All observations	118	-0.02	2.59

Table 4.3: Overview of the GOSAT-2 XCO_2 products vs TCCON co-located measurements. 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.

	Full Physics					
Variable	N	μ (ppm)	σ (ppm)	$\bar{\mu} \pm \sigma_{\bar{\mu}}$ (ppm)	$\bar{\sigma} \pm \sigma_{\bar{\sigma}}$ (ppm)	R
GOSAT2 Land	12557	-0.01	2.21	0.06 ± 0.50	2.28 ± 0.56	0.82
GOSAT-2 Ocean	118	-0.02	2.59	0.54 ± 1.31	2.39 ± 0.48	0.63

Figure 4.3 Comparison of land single soundings of XCO_2 from the full physics retrieval (blue circles) with co-located TCCON (pink triangles) measurements at all TCCON sites for the period Feb 2019 to Dec 2021. Histograms are also given for each station indicating the number of GOSAT-2 retrievals present throughout the time series.

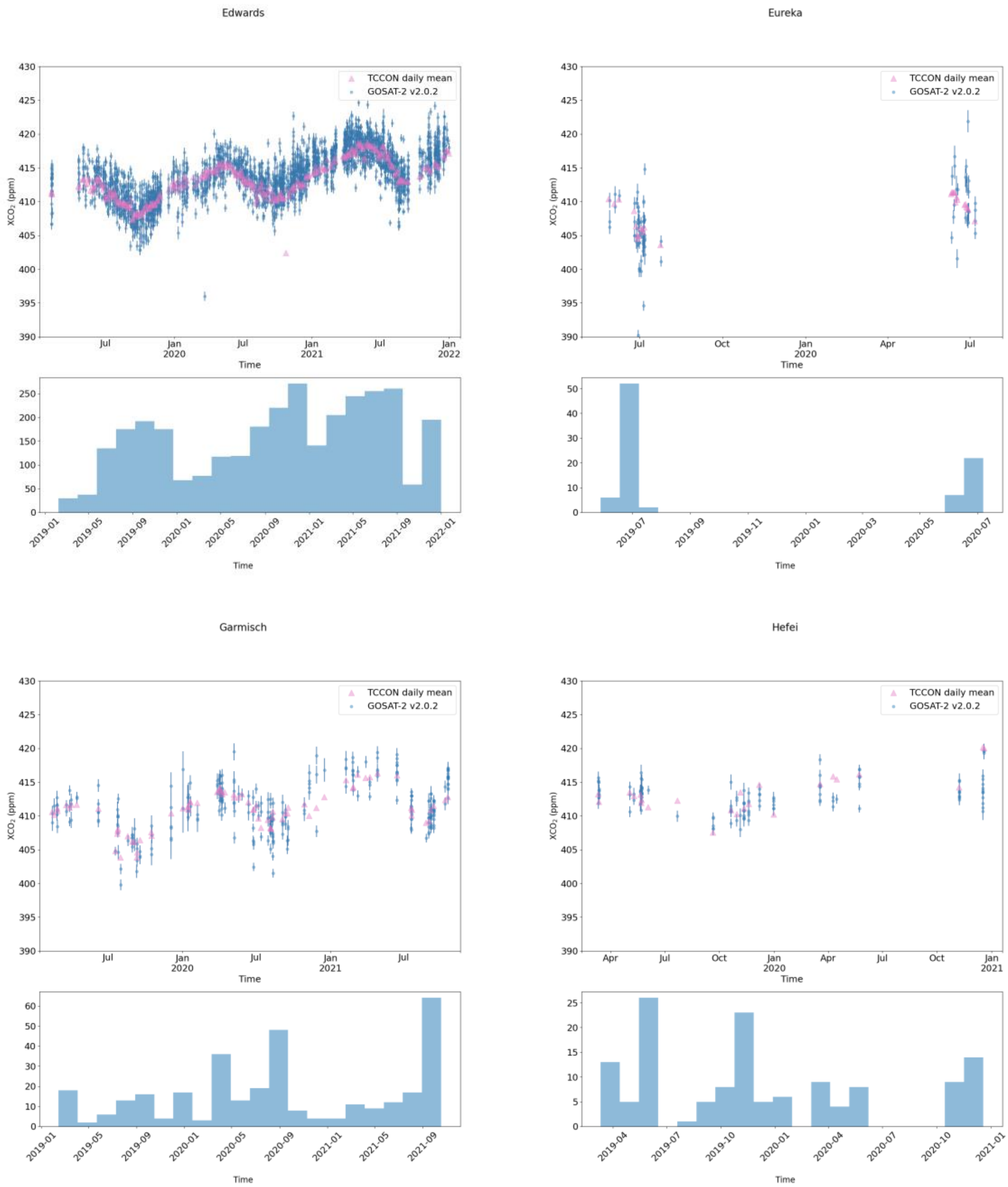

Figure 4.3 cont.

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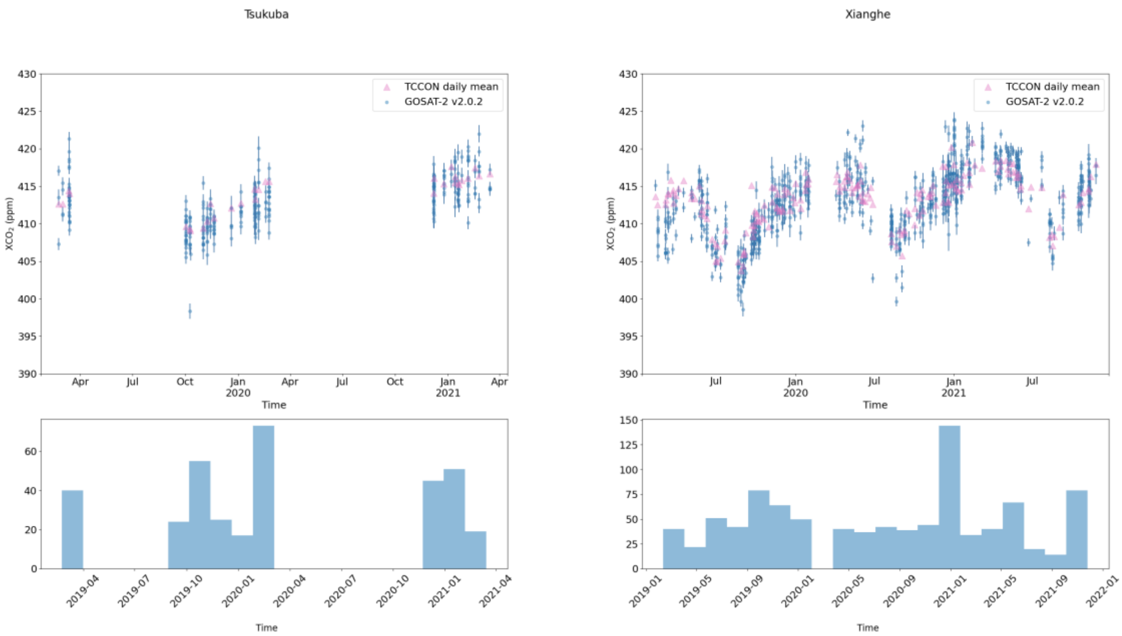

Figure 4.3 cont.

4.2 Overview GOSAT Statistics

Figure 4.4 shows a comparison of GOSAT-2 and GOSAT XCO_2 for the bias corrected product. Table 4.4 shows a summary of the corresponding statistics. The bias-correction of the 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 smaller than those found in the comparison with TCCON.

From Figure 4.4 and Table 4.4 it is clear that the correlation between GOSAT and GOSAT-2 for the XCO_2 v2.0.2 product is low. It is the case that a low correlation is observed for CO_2 compared to CH_4, however correlations coefficients of 0.3 for land and ocean measurements in v2.0.2 are lower than those presented in v2.0.0 (Krisna et al. 2022), who find correlation coefficients of 0.71 and 0.57 for bias corrected land and ocean measurements respectively.

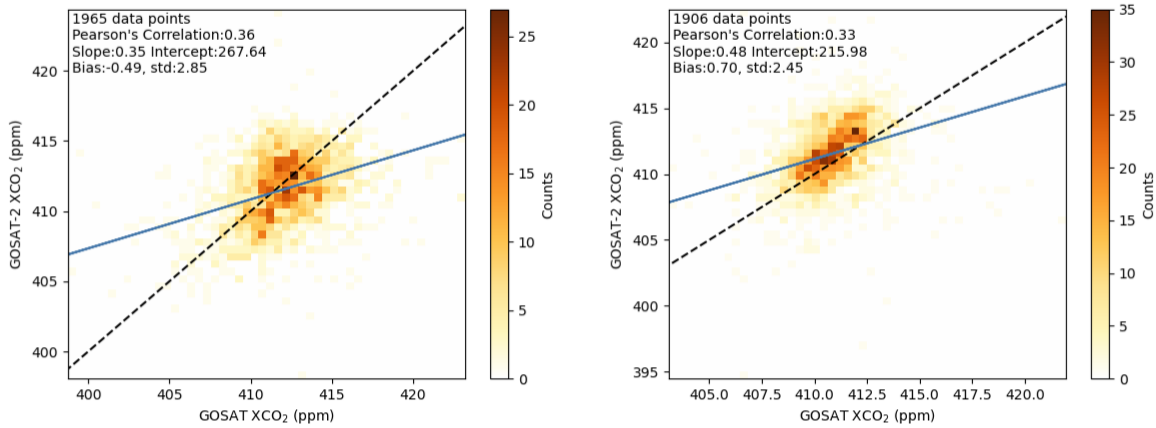

Figure 4.4: Comparison of land (left) and ocean (right) single soundings of XCO_2 with co-located GOSAT and GOSAT-2 measurements for the period Feb 2019 - Dec 2021.

Table 4.4. Summary of the comparison of full physics GOSAT vs GOSAT-2 for daily 2°x2° mean concentrations. Period covered is Feb 2019 to Dec 2021.

Land	N	R	µ (ppb)	σ (ppb)	Ocean	N	R	µ (ppm)	σ (ppm)
	1965	0.36	-0.49	2.85		1906	0.33	0.70	2.45

It should be noted that the XCO_2 v2.0.2 product shows a better correlation (R=0.82) with TCCON compared to v2.0.0 (R=0.75), implying that the data quality of v2.0.2 is better, considering that TCCON is the best reference for high quality data not GOSAT. This is enforced by the improvement in the spatial accuracy in v2.0.2, decreasing from 1.0 ppm in v2.0.0 to 0.5 ppm here.

The reason for the lower correlation between GOSAT and GOSAT-2 presented in this document is likely due to the different filtering techniques used in v2.0.2 and v.2.0.0 (Krisna et al. 2022). Here we apply a machine learning approach by implementing a random forest model to predict the quality of retrievals based on a selection of retrieval parameters, whereas in v2.0.0 post-processing quality filtering was performed using threshold filtering criteria, flagging data as bad quality whose retrieval parameters were outside a manually defined set of limits. This second kind of filtering technique is the same as has been applied to all previous SRON GOSAT and GOSAT-2 products. Therefore it is logical that that previous products - i.e. GOSAT-2 v.2.0.0 - would show a better correlation since they have applied the same quality filtering. This would explain the improved validation statistics with respect to TCCON in v2.0.2, as the random forest filtering technique performs better, while simultaneously explaining the deviation from a good correlation with 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 SRFP XCO_2 product, 2.36 for land retrievals and 3.24 for ocean retrievals and an uncertainty ratio of 0.83 and 0.82 for land and ocean, respectively.

The uncertainties in the product are already scaled and represented by the parameter "xco2_uncertainty". The unscaled values are added under the parameter name "raw_xco2_err".

5 Conclusions

This report summarizes the performance of the RemoTeC GOSAT-2 SRFP XCO_2 retrieval. In general, we find very good agreement with GOSAT 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 SRFP product. The standard deviation of the GOSAT-2 product presented here has improved compared to the SRFP XCO_2 product from C3S v2.0.0 by 0.56 ppm.

The correlation of GOSAT-2 and TCCON has improved compared to v2.0.0 (Krisna et al. 2022) to 0.82 while the correlation with GOSAT has decreased. This may be attributed to the different filtering techniques applied, where a machine learning approach is implemented in v2.0.2 in contrast to a strict threshold filtering method in v2.0.0. The approach using the random forest model results in better data quality, evident by the improved validation statistics with respect to TCCON.

The spatial accuracy (standard deviation site biases) is 0.5 ppm, which has improved by a factor of 2 compared to v2.0.0 (Krisna et al. 2022), and a single measurement precision of around 2.2 ppm is observed.

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