Product Quality Assessment Report (PQAR) – ANNEX C for product CH4_GO2_SRPR (v2.0.1, 2019-2022)

C3S2_312a_Lot2_DLR – Atmosphere

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History of modifications

Version	Date	Description of modification	Chapters / Sections
1.1	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: Primarily correction of typos.	All
4.0	18-August-2020	Update for CDR4 (2009-2019)	All
5.0 beta	18-February-2021	Update for CDR5 (2009-mid2020)	All
5.0	23-April-2021	Minor improvements after review by Assimila	All
6.0	04-August-2022	Update for CDR6: GOSAT-2 retrievals (2019 – 2021)	All
6.1	14-December-2022	Update after review (use of new template, several improvements at various places)	All
6.2	14-February-2023	Update after 2nd review. Several improvements at various places.	All
6.3	02-March-2023	Minor update after 2nd review to generate clean version.	All
7.0	24-August-2023	Update of version to v2.0.1 which implements updated models for XCO_2 used in proxy calculation	All
7.1	19-September-2023	Update after review	All
7.2	17-November-2023	Minor update after review	All

List of datasets covered by this document

Deliverable ID	Product title	Product type (CDR, ICDR)	Version number	Delivery date
WP2-FDDP-GHG-v2	CH4_GO2_SRPR	CDR 7	2.0.1	31-Aug-2023

Related documents

Reference ID	Document
D1	**Main PQAR:** Buchwitz, M., et al., Product Quality Assessment Report (PQAR) – Main document for Greenhouse Gas (GHG: CO_2 & CH_4) data set CDR 7 (2003-2022), project C3S2_312a_Lot2_DLR – Atmosphere, 2023. *Important Note:* *This document is an ANNEX to the Main PQAR document and contains the quality assessment results of the data provider.* ***For the final overall quality assessment results of the data products described in this document see the Main PQAR document.***
D2	**TRD GAD GHG, 2021:** Buchwitz, M., Reuter, M., Schneising-Weigel, O., Aben, I., Wu, L., Hasekamp, O. P., Boesch, H., Di Noia, A., Crevoisier, C., Armante, R.: Target Requirement and Gap Analysis Document, Copernicus Climate Change Service (C3S) project on satellite-derived Essential Climate Variable (ECV) Greenhouse Gases (CO_2 and CH_4) data products, Version 3.1, 19-February-2021, pp. 81, 2021. Latest version: http://wdc.dlr.de/C3S_312b_Lot2/Documentation/GHG/C3S2_312a_Lot2_TRD-GAD_GHG_latest.pdf

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
GOSAT-2	Greenhouse Gases Observing Satellite 2
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
RemoTeC	Retrieval algorithm developed at SRON
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
TANSO-FTS-2	Fourier Transform Spectrometer on GOSAT-2
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

Essential climate variable (ECV)

An ECV is a physical, chemical, or biological variable or a group of linked variables that critically contributes to the characterization of Earth's climate.

Climate data record (CDR)

The US National Research Council (NRC) defines a CDR as a time series of measurements of sufficient length, consistency, and continuity to determine climate variability and change.

Fundamental climate data record (FCDR)

A fundamental climate data record (FCDR) is a CDR of calibrated and quality-controlled data designed to allow the generation of homogeneous products that are accurate and stable enough for climate monitoring.

Thematic climate data record (TCDR)

A thematic climate data record (TCDR) is a long time series of an essential climate variable (ECV).

Intermediate climate data record (ICDR)

An intermediate climate data record (ICDR) is a TCDR which undergoes regular and consistent updates, for example because it is being generated by a satellite sensor in operation.

Satellite data processing levels

The NASA Earth Observing System (EOS) distinguishes six processing levels of satellite data, ranging from Level 0 (L0) to Level 4 (L4) as follows.

L0   Unprocessed instrument data

L1A   Unprocessed instrument data alongside ancillary information

L1B   Data processed to sensor units (geo-located calibrated spectral radiance and solar irradiance)

L2   Derived geophysical variables (e.g., XCO_2) over one orbit

L3   Geophysical variables averaged in time and mapped on a global longitude/latitude horizontal grid

L4   Model output derived by assimilation of observations, or variables derived from multiple measurements (or both)

Additional definitions as relevant for this document:

In the following some relevant Target Requirement (TR) related definitions are given. For details please see TRD (D2), 2017, ESA-CCI-GHG-URDv2.1 and CMUG-RBD, 2010:

Systematic error: component of measurement error that in replicate measurements remains constant or varies in a predictable manner

Note: "Systematic error" = "Absolute systematic error" (in contrast to "Relative systematic error" defined below).

For satellite GHG ECV products especially the "Relative systematic error" is important. The definition as used here is as follows:

Relative systematic error: Identical with "Systematic error" but after bias correction and without considering a possible "global offset" (overall mean bias). Reflects the importance of spatially and temporally correlated errors ("spatio-temporal biases"). Computed from standard deviations of spatial and temporal biases.

Bias: estimate of a systematic measurement error (JCGM, 2008).

Precision is the measure of reproducibility or repeatability of the measurement without reference to an international standard so that precision is a measure of the random and not the systematic error. Suitable averaging of the random error can improve the precision of the measurement but does not establish the systematic error of the observation (CMUG-RBD, 2010).

Note: Precision (as explained in *TRD (D2)*) is quantified with the standard deviation (1-sigma) of the error distribution.

Stability is a term often invoked with respect to long-term records when no absolute standard is available to quantitatively establish the systematic error - the bias defining the time-dependent (or instrument-dependent) difference between the observed quantity and the true value (CMUG-RBD, 2010).

Note: Stability requirements cover inter-annual error changes. If the change in the average bias from one year to another is larger than the defined values, the corresponding product does not meet the stability requirement.

Representativity is important when comparing with or assimilating in models. Measurements are typically averaged over different horizontal and vertical scales compared to model fields. If the measurements are smaller scale than the model it is important. The sampling strategy can also affect this term (CMUG-RBD, 2010).

Threshold requirement: The threshold is the limit at which the observation becomes ineffectual and is not of use for climate-related applications (CMUG-RBD, 2010).

Goal requirement: The goal is an ideal requirement above which further improvements are not necessary (CMUG-RBD, 2010).

Breakthrough requirement: The breakthrough is an intermediate level between the "threshold" and "goal" requirements, which - if achieved - would result in a significant improvement for the targeted application. The breakthrough level may be considered as an optimum, from a cost-benefit point of view when planning or designing observing systems (CMUG-RBD, 2010).

Horizontal resolution is the area over which one value of the variable is representative of (CMUG-RBD, 2010).

Vertical resolution is the height over which one value of the variable is representative of. Only used for profile data (CMUG-RBD, 2010).

Observing Cycle (or **Revisit Time)** is the temporal frequency at which the measurements are required (CMUG-RBD, 2010).

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Scope of document

This document is a Product Quality Assessment Report (PQAR) for the Copernicus Climate Change Service (C3S, https://climate.copernicus.eu/) greenhouse gas (GHG) component as covered by project C3S2_312a_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 validation / quality assessment of C3S2 product CH4_GO2_SRPR v2.0.1.

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

Executive summary

This report summarizes the performance of the RemoTeC CH4_GO2_SRPR retrievals. In general, we find very good agreement with TCCON data for both land and sunglint modes. All have a very high degree of correlation with TCCON (R>0.8).

The station-to-station bias is 2.77 ppb and a standard deviation of around 18.09 ppb is observed for most TCCON stations. We also checked the stability of the bias over time as the GOSAT time series now spans a period of almost 4 years and found that there has been no significant change in the bias over time, indicating a very good detector stability. We achieved both Target Requirements (TR) for accuracy and stability with 99 % for and 99 % probabilities, respectively.

1. Product validation methodology

Validation of the CH4_GO2_SRPR v2.0.1 is performed by comparison with a selection of ground-based Fourier Transform Spectrometer (FTS) Total Carbon Column Observing Network (TCCON) stations. These TCCON data provide total column XCH_4 measurements that are used to filter our retrievals and perform a bias correction of our data product. The final filtered and bias corrected product is then compared to TCCON to evaluate the global bias, accuracy and systematic biases (spatial and temporal) in the retrievals. In this validation the TCCON GGG2020 (Laughner et al. 2021) official release has been used.

1.1 Co-location method

We co-locate the GOSAT-2 soundings with the TCCON measurements using the following criteria:
- GOSAT-2 sounding within ±5 degree latitude and ±8 degree longitude of TCCON station
- GOSAT-2 sounding within ±2 hours of TCCON measurements

We then average all the TCCON measurements within ±2 hours of a GOSAT measurement to create a set of GOSAT-2-TCCON pairs. These co-located pairs are then used to perform the validation procedure.

Sunglint 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. As a result, only TCCON stations that are close to shorelines or on islands have collocated sunglint measurements with GOSAT-2.

2. Validation Results

2.1 TCCON Validation CH4_GO2_SRPR

2.1.1 Validation

Figure 1 shows a very strong correlation of the retrieved (bias-corrected) XCH_4 with the TCCON XCH_4 (r > 0.8). This gives us confidence that our bias correction based on the retrieved albedo works correctly and takes out most of the bias.

Figure 2 shows in detail for each station the remaining bias and standard deviation for the co-located GOSAT soundings.

In the case of land soundings, the station-to-station standard deviation is 2.77 ppb. Caltech/Edwards shows the largest number of co-locations for land measurements. All stations show a residual bias of less than 7.5 ppb, except for Rikubetsu and Eureka which has a remaining bias of ~10 ppb. For sunglint mode, the correlation with TCCON is very high (R=0.92).

Figure 3 presents Hovmöller diagrams of XCH_4 as well as the uncertainty on this parameter, along with the number of observations across the range of GOSAT-2 observations.

Figure 1: Validation of XCH$_4$ retrieved by GOSAT-2-RemoTeC with ground based TCCON measurements for land (top) and sunglint (bottom) soundings. N indicates the number of GOSAT-2-TCCON colocations, μ is the average difference (for individual measurements) between GOSAT-2 and TCCON, σ the standard deviation of the GOSAT-2 TCCON difference (for individual measurements) and R the Pearson's correlation coefficient between the two set of observations.
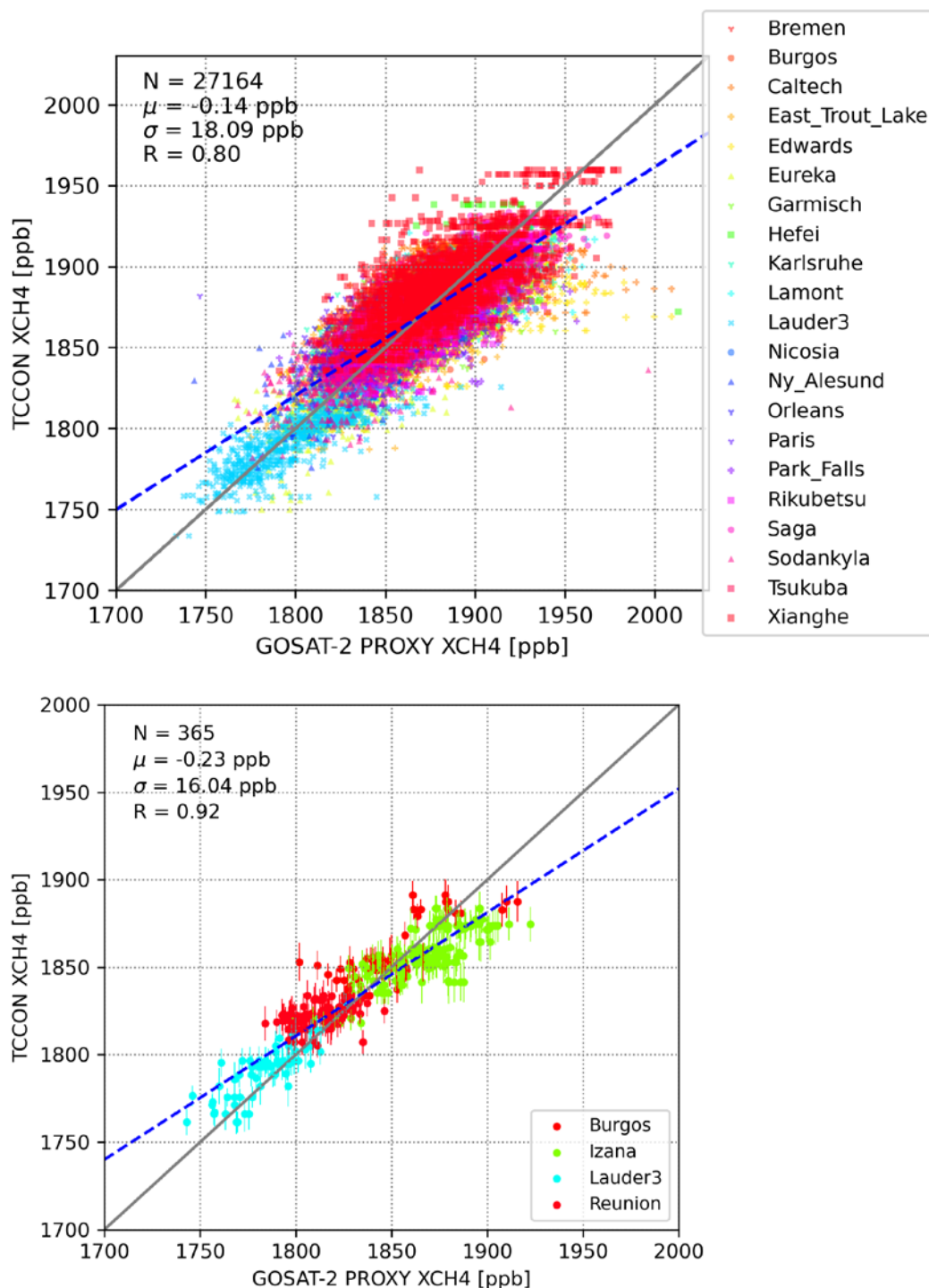
Figure 2: The bias, standard deviation and number of measurements per station for land (left) and sunglint (right) soundings for the period between the year 2019 and 2022.
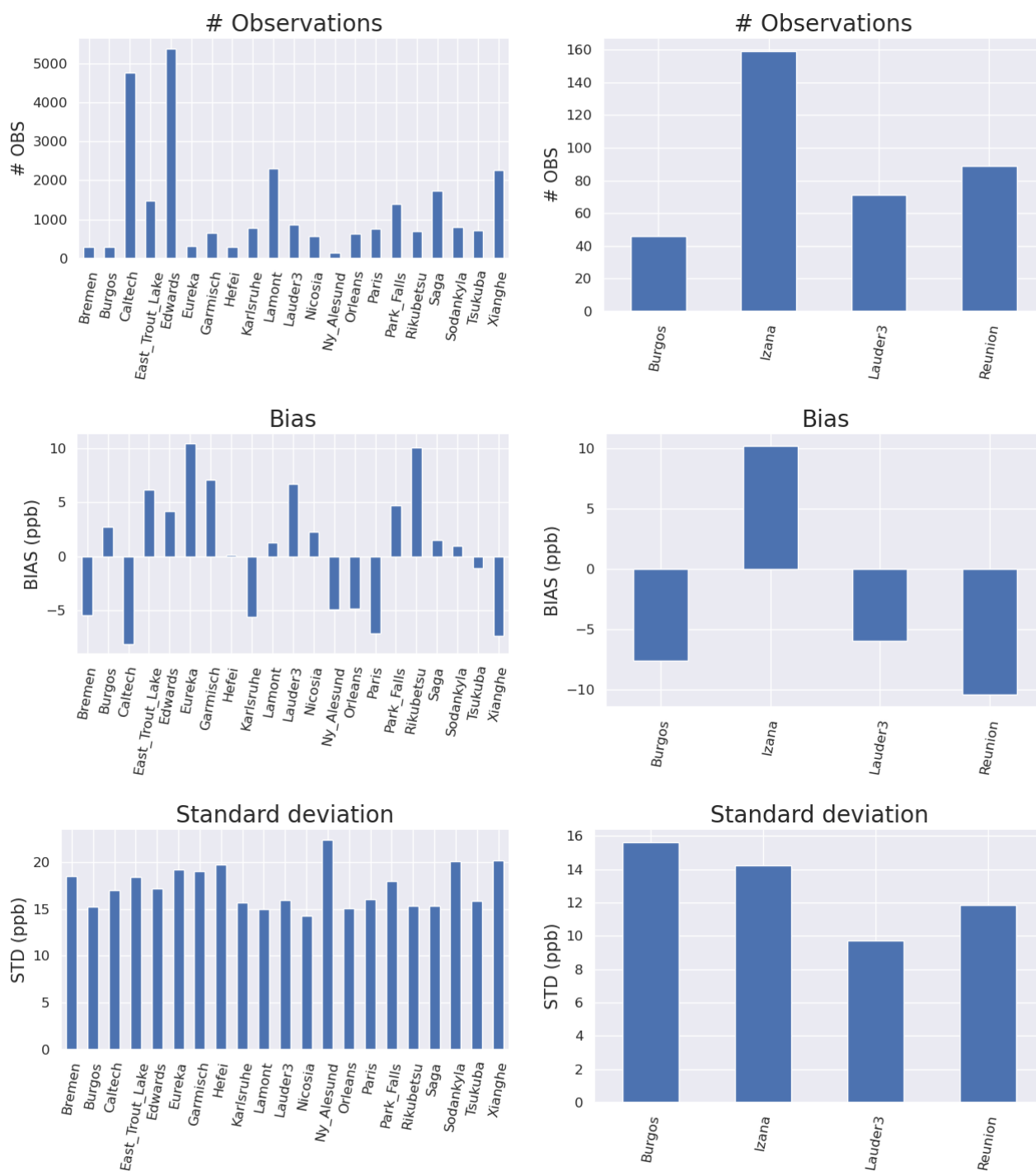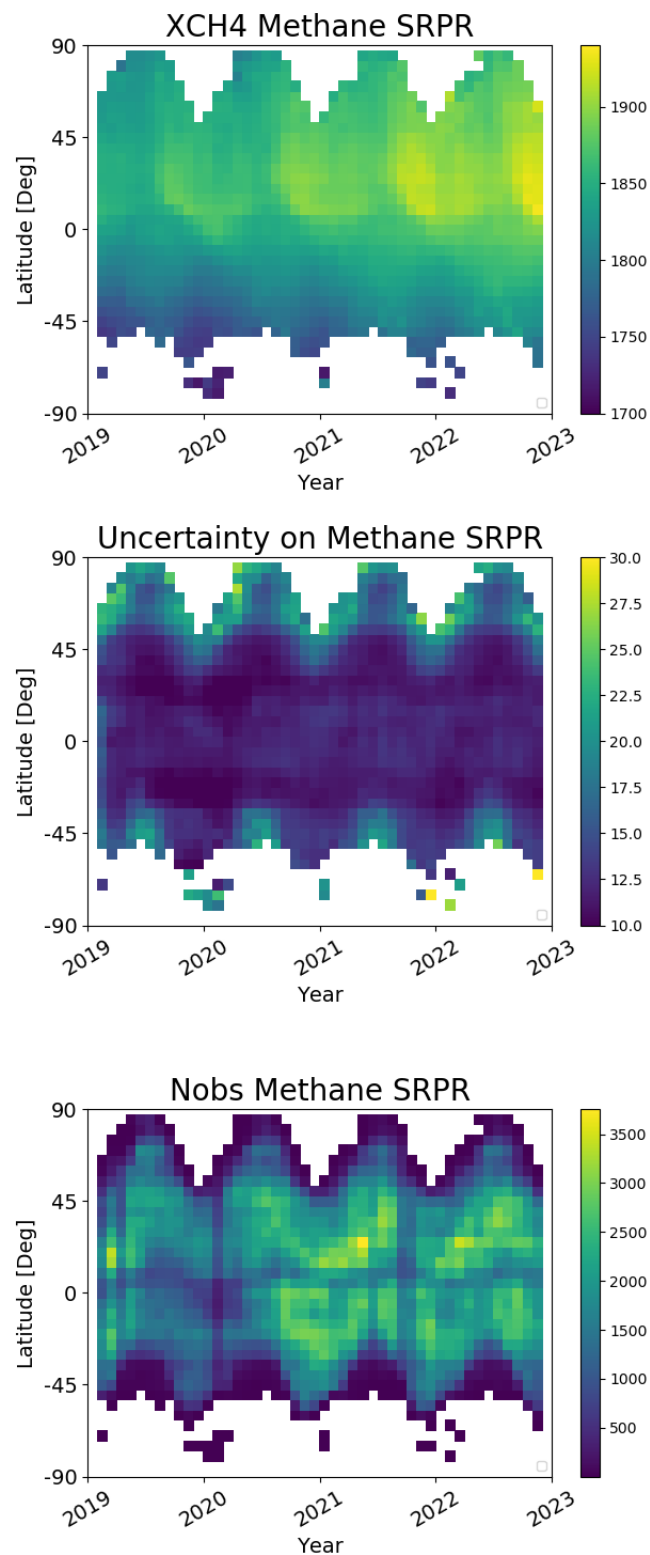
Figure 3: The CH4_GO2_SRPR global dataset in slices of 10 degrees latitude as a function of time. The increase in XCH$_4$ concentrations during the last couple of years can clearly be seen. The date range covered is the full GOSAT-2 sample (Feb 2019 – end Dec 2022).

2.1.2 Stability

Stability (both linear and year-to-year variability) is an essential part of the validation and can reveal potential degradation or other time-dependent effects in the GOSAT-2 data products.
Figure 4 and Figure 5 show the time series for the individual stations. As can be seen the time coverage for different stations can differ significantly and occasionally gaps occur due to maintenance of the TCCON station.

To determine the linear stability, we add all co-located TCCON measurements together and fit a linear relation to the remaining bias as a function of time. The year-to-year bias variability is the difference between the minimum of the bias in one year versus the maximum of the bias in one year. The results are shown in Table 2.

Figure 4: *Upper panels:* Timeseries for the individual stations for land soundings for CH4_GO2_SRPR. The pink triangles represent the daily average XCH$_4$ of the TCCON data and the blue circles are all the retrieved GOSAT-2 data. *Lower panels:* Histogram of number of GOSAT-2 retrievals in bins over the time range in question.
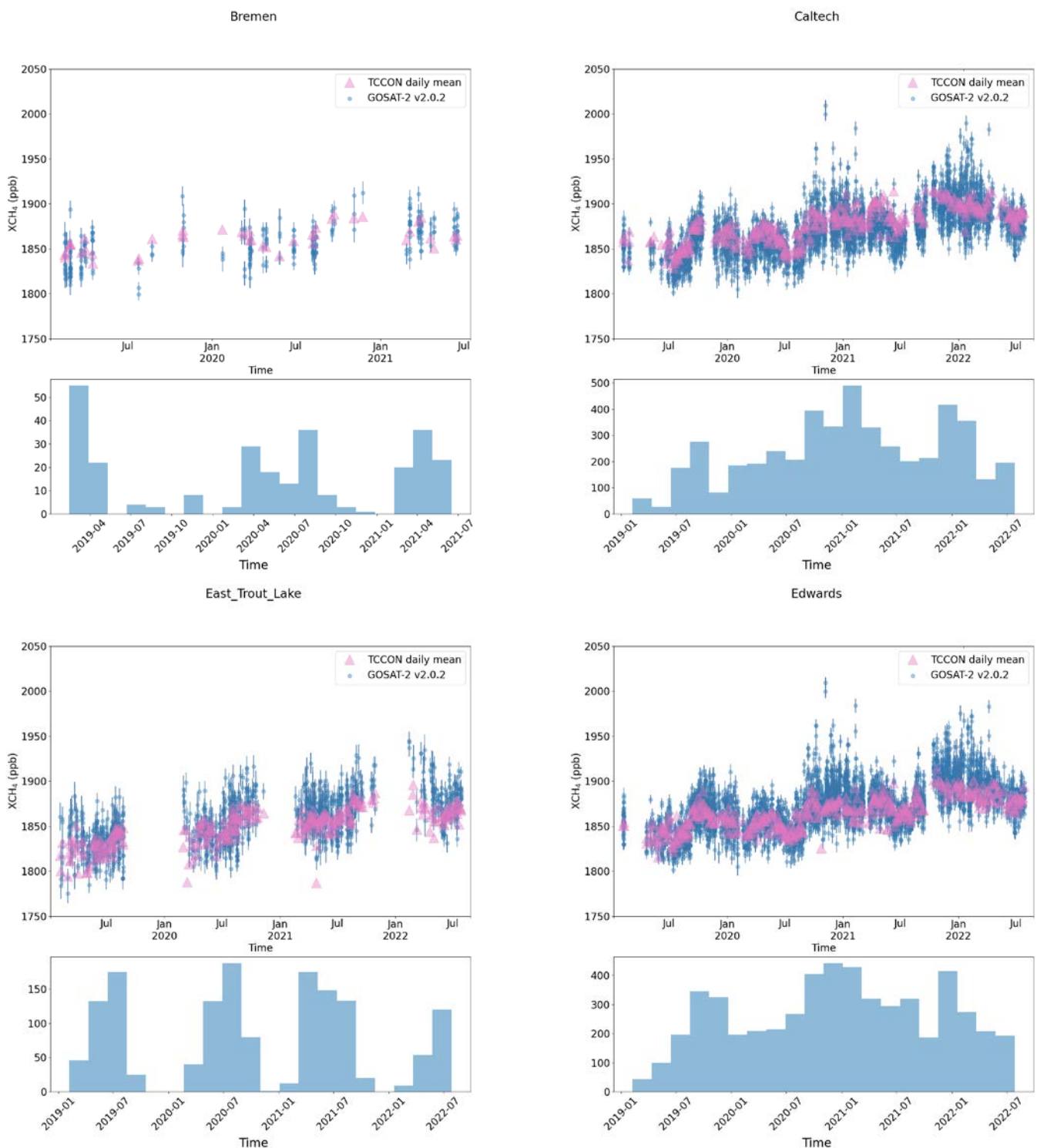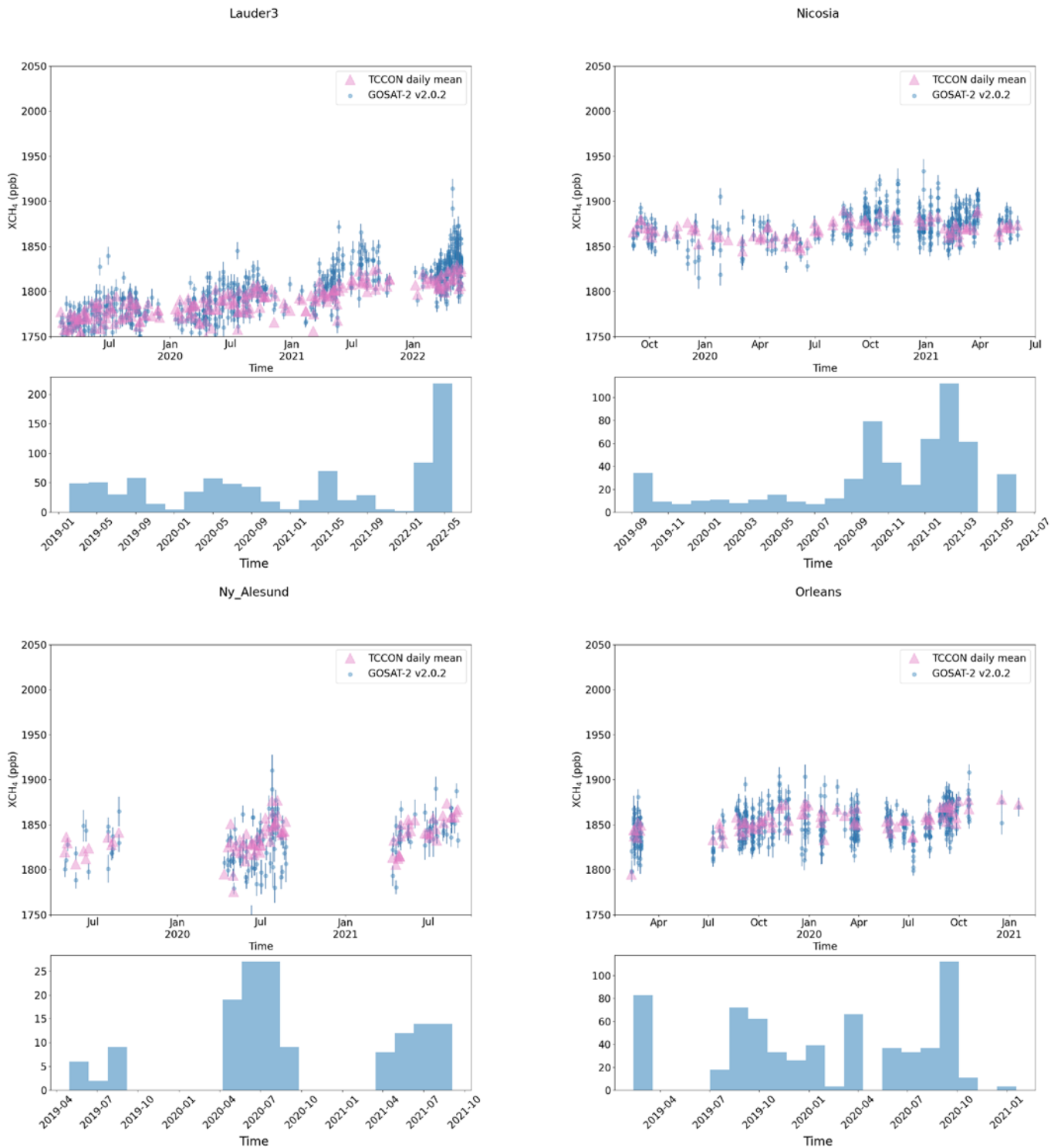
Figure 4 cont.

Figure 4 cont.
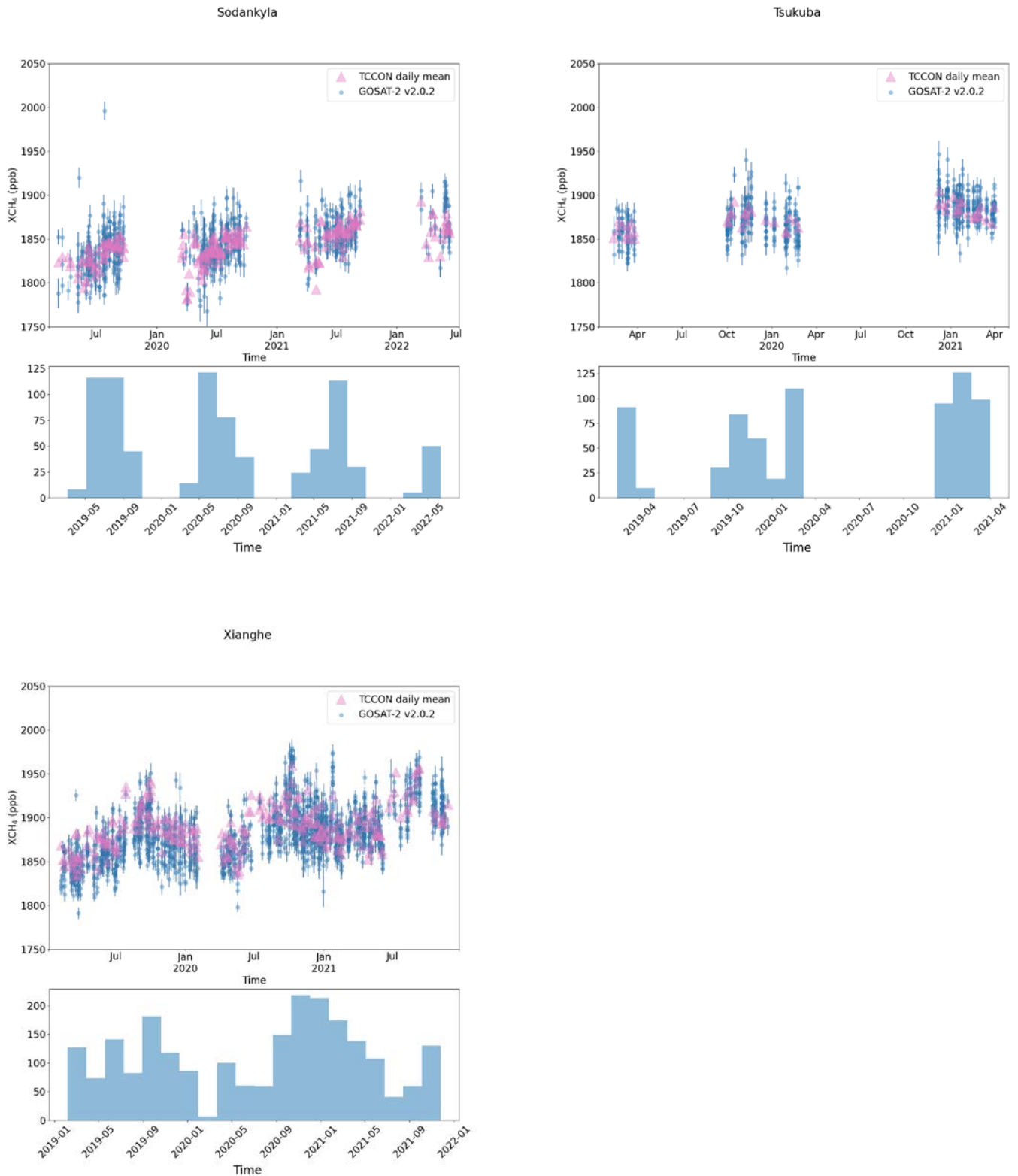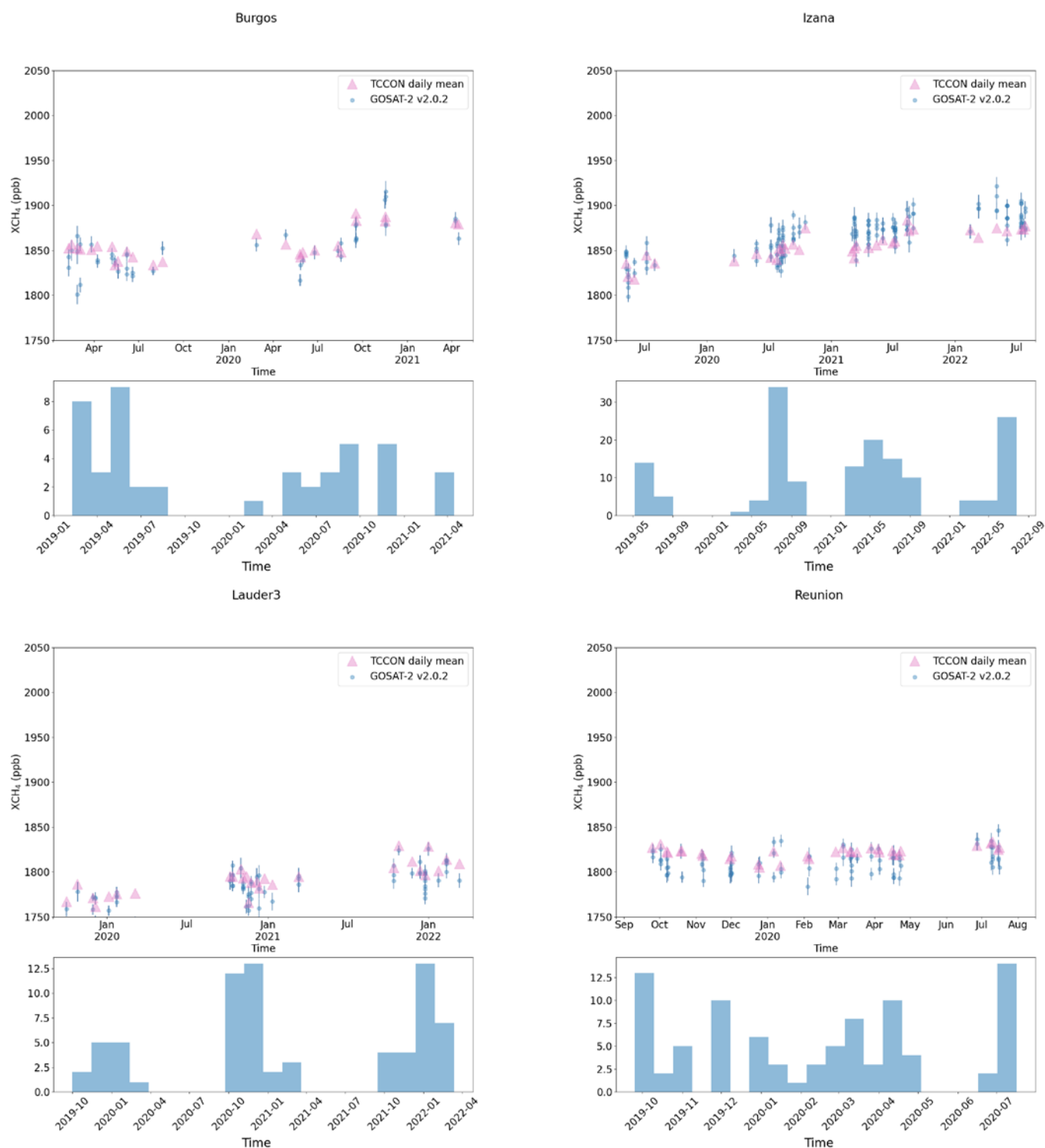
Figure 4 cont.

Figure 4 cont.

Figure 5: *Upper panels:* Timeseries for the individual stations for ocean soundings for CH4_GO2_SRPR. The pink triangles represent the daily average XCH_4 of the TCCON data and the blue circles are all the retrieved GOSAT-2 data. *Lower panels:* Histogram of number of GOSAT-2 retrievals in bins over the time range in question.

2.1.3 Validation summary

The validation results are summarized in the table below.

Table 2: Product Quality Summary Table for product CH4_GO2_SRPR. T, B and G refer to threshold, breakthrough and goal, respectively.

Parameter [unit]	Achieved performance	Requirement	TR	Comments
Product Quality Summary Table for Product: CH4_GO2_SRPR Level: 2, Version: 2.0.1, Time period covered: 02.2019 – 12.2022				
Single measurement precision (1-sigma) in [ppb]	18.09	< 34 (T) < 17 (B) < 9 (G)	-	-
Uncertainty ratio) in [-]: Ratio reported uncertainty to standard deviation of satellite-TCCON difference	0.78	-	-	No requirement but value close to unity expected for a high quality data product.
Mean bias [ppb]	-0.14	-	-	No requirement but value close to zero expected for a high quality data product.
Accuracy: Relative systematic error [ppb]	Spatial: 2.1 +/- 0.26 Spatiotemporal: 2.77 +/- 2.40	< 10	Probability that accuracy TR is met: 99 %	-
Stability: Linear bias trend [ppb/year]	0.84 +/- 0.22 (1-sigma)	< 3	Probability that stability TR is met: 99 %	-
Stability: Year-to-year bias variability [ppb/year]	8.33 +/- 3.11 (1-sigma)	< 3	-	-

2.2 GOSAT-GOSAT2 Intercomparison

In this section we report on the comparison of the GOSAT-2 SRPR XCH4 data versus co-located GOSAT-1. Figure 6 shows a comparison of GOSAT-2 and GOSAT SRPR-CH4 for both the non-corrected and bias-corrected product. Table 3 shows a summary of the corresponding statistics. The bias-correction of observations has been performed with TCCON observations as described in the previous section. Overall, the products from the two satellites compare fairly well with relatively small biases, high correlations, and standard deviations smaller than those found in the comparison with TCCON. The bias-corrected comparison shows a better bias and standard deviation than the non-corrected version. This gives us confidence that the bias correction with performs well. In the bias corrected comparison, sunglint soundings show a higher residual bias between GOSAT and GOSAT-2 compared to land soundings. This is potentially due to the small number of TCCON sites with available data for sunglint measurements compared to land measurements.

Figure 6: Comparison of land and glint single soundings of SRPR-CH4 with co-located GOSAT and GOSAT-2 measurements for the period 2019-2022, for bias corrected and non-bias corrected data. Bias and standard deviation values are given in ppb.
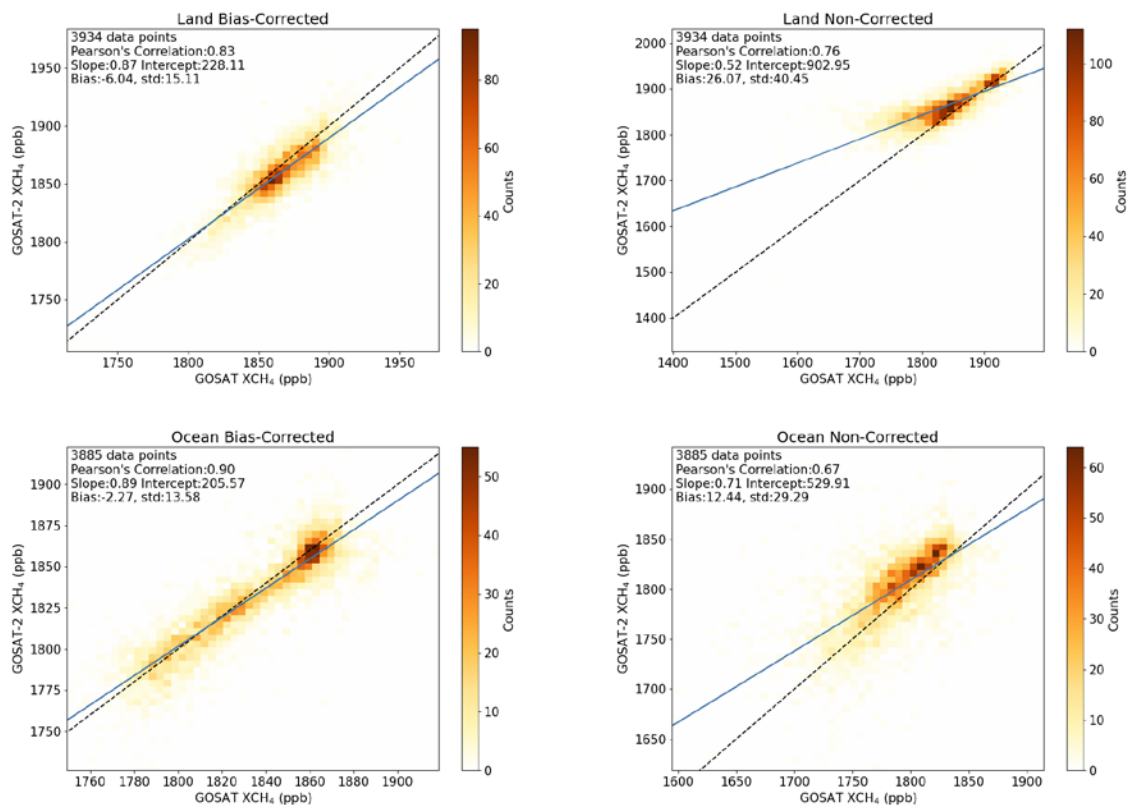
Table 3: Summary of the comparison of SRPR-CH$_4$ GOSAT vs GOSAT-2 for daily 1°x1° mean concentrations. Period covered is Feb 2019 to Dec 2022. The bias, standard deviation (precision), Pearson's correlation coefficient and number of observations (N) are given, for both the bias corrected and non-bias corrected values in land and glint mode.

Parameter	Land		Glint	
	Bias-Corrected	Non-corrected	Bias-Corrected	Non-Corrected
N	3934	3934	3885	3885
Correlation	0.83	0.76	0.90	0.67
Bias [ppm]	-6.04	26.07	-2.27	12.44
Single measurement prescision in ppm (std)	15.11	40.45	13.58	29.29

3. Application(s) specific assessments

No application specific assessments have been carried out.

4. Compliance with user requirements

For the CH4_GO2_SRPR product we achieved 99 % for TR's Accuracy and 87 % for TR's Stability

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