



Product Quality Assessment Report (PQAR) – ANNEX C for product CH4_GOS_SRPR (v2.3.9, 2009-mid2020)

C3S_312b_Lot2_DLR – Atmosphere

Issued by: Lianghai Wu, SRON, The Netherlands

Date: 23/04/2021

Ref: C3S_D312b_Lot2.2.3.2-v3.0_PQAR-GHG_ANNEX-C_v5.0

Official reference number service contract: 2018/C3S_312b_Lot2_DLR/SC1



This document has been produced in the context of the Copernicus Climate Change Service (C3S). The activities leading to these results have been contracted by the European Centre for Medium-Range Weather Forecasts, operator of C3S on behalf of the European Union (Delegation Agreement signed on 11/11/2014). All information in this document is provided "as is" and no guarantee or warranty is given that the information is fit for any particular purpose. The user thereof uses the information at its sole risk and liability. For the avoidance of all doubts, the European Commission and the European Centre for Medium-Range Weather Forecasts has no liability in respect of this document, which is merely representing the authors view.



Contributors

**INSTITUTE OF ENVIRONMENTAL PHYSICS (IUP),
UNIVERSITY OF BREMEN, BREMEN, GERMANY
(IUP)**

M. Buchwitz

**SRON NETHERLANDS INSTITUTE FOR SPACE RESEARCH,
UTRECHT, THE NETHERLANDS
(SRON)**

I. Aben

L. Wu

O. P. Hasekamp



Table of Contents

History of modifications	5
Related documents	6
Acronyms	7
General definitions	9
Scope of document	10
Executive summary	11
1. Product validation methodology	12
1.1 Co-location method	12
2. Validation Results	15
2.1 Product CH₄_GOS_SRPR	15
2.1.1 Validation	15
2.1.2 Stability	18
2.1.3 Validation summary	22
3. Application(s) specific assessments	23
4. Compliance with user requirements	23
References	24



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



Related documents

Reference ID	Document
D1	<p>Main PQAR:</p> <p>Buchwitz, M., et al., Product Quality Assessment Report (PQAR) – Main document for Greenhouse Gas (GHG: CO₂ & CH₄) data set CDR 5 (01.2003-06.2020), project C3S_312b_Lot2_DLR – Atmosphere, v5.0, 2021.</p> <p>Important Note:</p> <p><i>This document is an ANNEX to the Main PQAR document and contains the quality assessment results of the data provider.</i></p> <p><i>For the final overall quality assessment results of the data products described in this document see the Main PQAR document.</i></p>



Acronyms

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



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



General definitions

Table 1 lists some general definitions relevant for this document.

Table 1: General definitions.

Item	Definition
XCO ₂	Column-averaged dry-air mixing ratios (mole fractions) of CO ₂
XCH ₄	Column-averaged dry-air mixing ratios (mole fractions) of CH ₄
L1	Level 1 satellite data product: geolocated radiance (spectra)
L2	Level 2 satellite-derived data product: Here: CO ₂ and CH ₄ information for each ground-pixel
L3	Level 3 satellite-derived data product: Here: Gridded CO ₂ and CH ₄ information, e.g., 5 deg times 5 deg, monthly
L4	Level 4 satellite-derived data product: Here: Surface fluxes (emission and/or uptake) of CO ₂ and CH ₄



Scope of document

This document is a Product Quality Assessment Report (PQAR) for the Copernicus Climate Change Service (C3S, <https://climate.copernicus.eu/>) greenhouse gas (GHG) component as covered by project C3S_312b_Lot2.

Within this project satellite-derived atmospheric carbon dioxide (CO₂) and methane (CH₄) 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 CO₂ and CH₄, denoted XCO₂ (in parts per million, ppm) and XCH₄ (in parts per billion, ppb), respectively.
- Mid/upper tropospheric mixing ratios of CO₂ (in ppm) and CH₄ (in ppb).

This document describes the validation / quality assessment of C3S product CH4_GOS_SRPR.

These products are XCO₂ and XCH₄ Level 2 products as retrieved from GOSAT using algorithms developed at SRON, The Netherlands.



Executive summary

This report summarizes the performance of the RemoTeC CH₄_GOS_SRPR retrievals. In general, we find very good agreement with TCCON data for all three modes (gain H, gain M and sunglint). All have a very high degree of correlation with TCCON ($R \sim 0.9$).

The station to station bias is 2.75 ppb and a standard deviation of around 14.47 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 11 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 Requirement (TR) requirements for accuracy and stability with 100 % in both cases.



1. Product validation methodology

Validation of the CH₄_GOS_SRPR is performed by comparison a selection of ground-based FTS TCCON stations. These provide total column XCH₄ 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, retrieval accuracy and systematic biases (spatial and temporal) in the retrievals. In this validation the TCCON GGG2014 official release has been used.

1.1 Co-location method

We co-locate the GOSAT soundings with the TCCON measurements using the following criteria:

- GOSAT sounding within ± 5 latitude and ± 8 longitude of TCCON station
- GOSAT sounding within ± 2 hours of TCCON measurements

In previous studies we have also employed a dynamic co-location method, based on a TM5-4DVAR forward model run. This essentially compares the modeled CO₂ concentration at a GOSAT sounding and the TCCON site and co-locates the soundings if the CO₂ concentrations are within 0.25 (or 0.5) ppm of each other. This is then used as a tracer for atmospheric transport. However, at the time of validating this dataset the dynamic co-locations for the newest year were not yet available. We therefore decided to use a box filter instead as we did want to include the newest year's data in our validation and wanted the whole dataset to have a consistent method for co-locating the GOSAT soundings.

We then average all the TCCON measurements within ± 2 hours of a GOSAT measurement to create a set of GOSAT-TCCON pairs. These co-located pairs are then used to perform the validation procedure. Figure 1-3 shows the co-located example soundings for the gain H, gain M and sunglint stations respectively.

Figure 1: GOSAT co-located example soundings for each TCCON station for gain H soundings. The map shows the elevation with dark green being low elevations and light green showing elevated areas. The blue stars show the location of the TCCON site, while the red dots are co-located GOSAT soundings. Top to down (left column) stations: Bialystok, Darwin, Karlsruhe, Orleans, Saga, Wollongong. Top to down (right column) stations: Bremen, Garmisch, Lamont, Park Falls, Sodankyla.

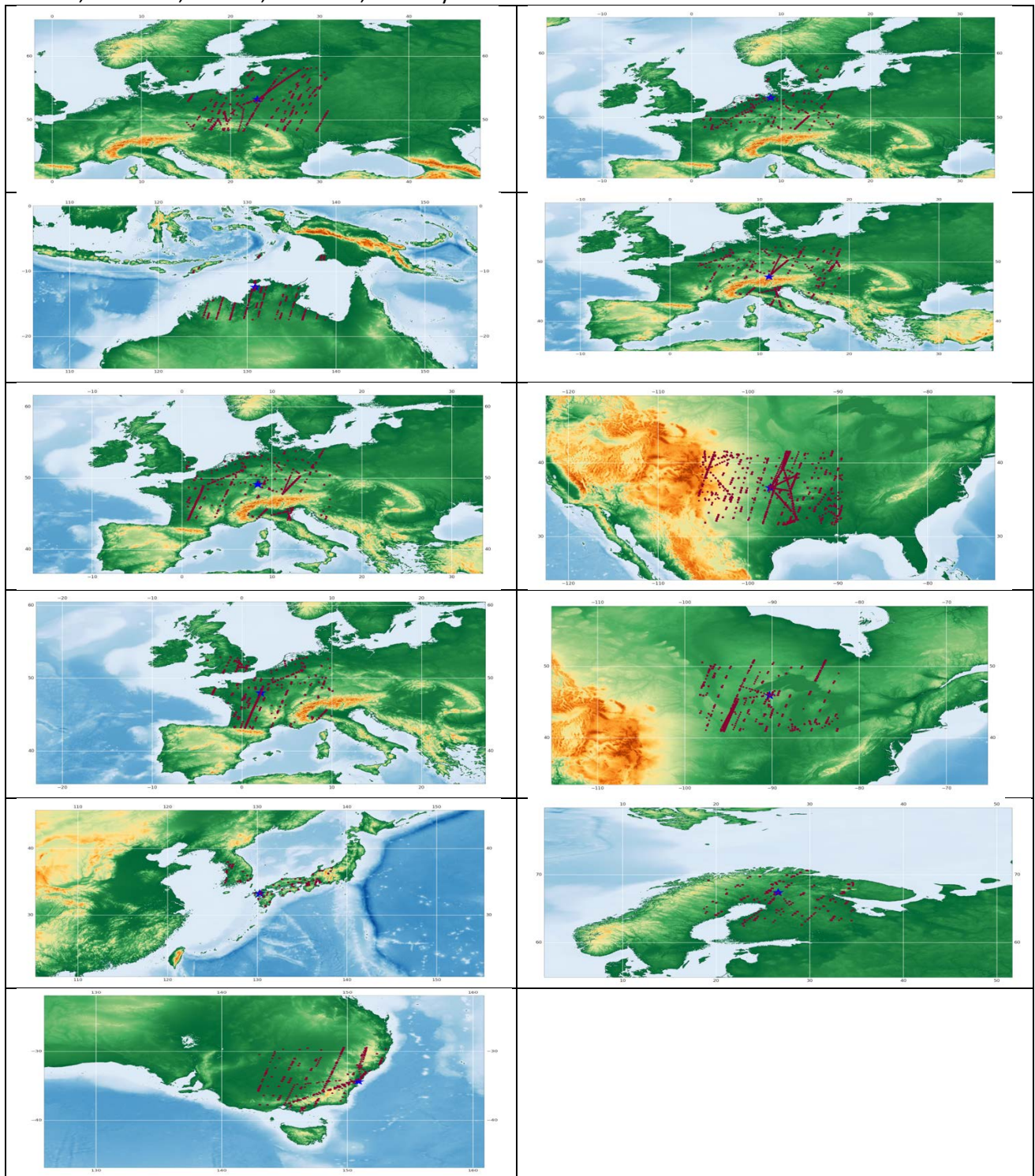




Figure 2: As Fig 1 but for gain M soundings. Stations are Dryden (left) and Wollongong (right).

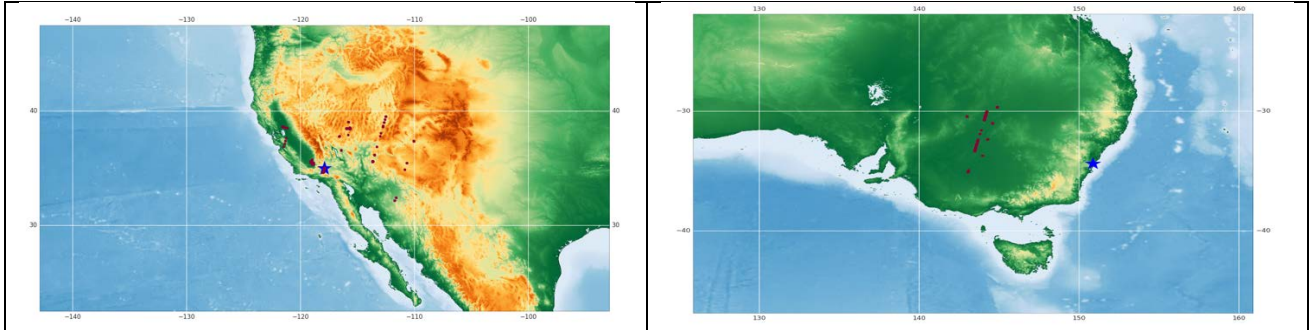
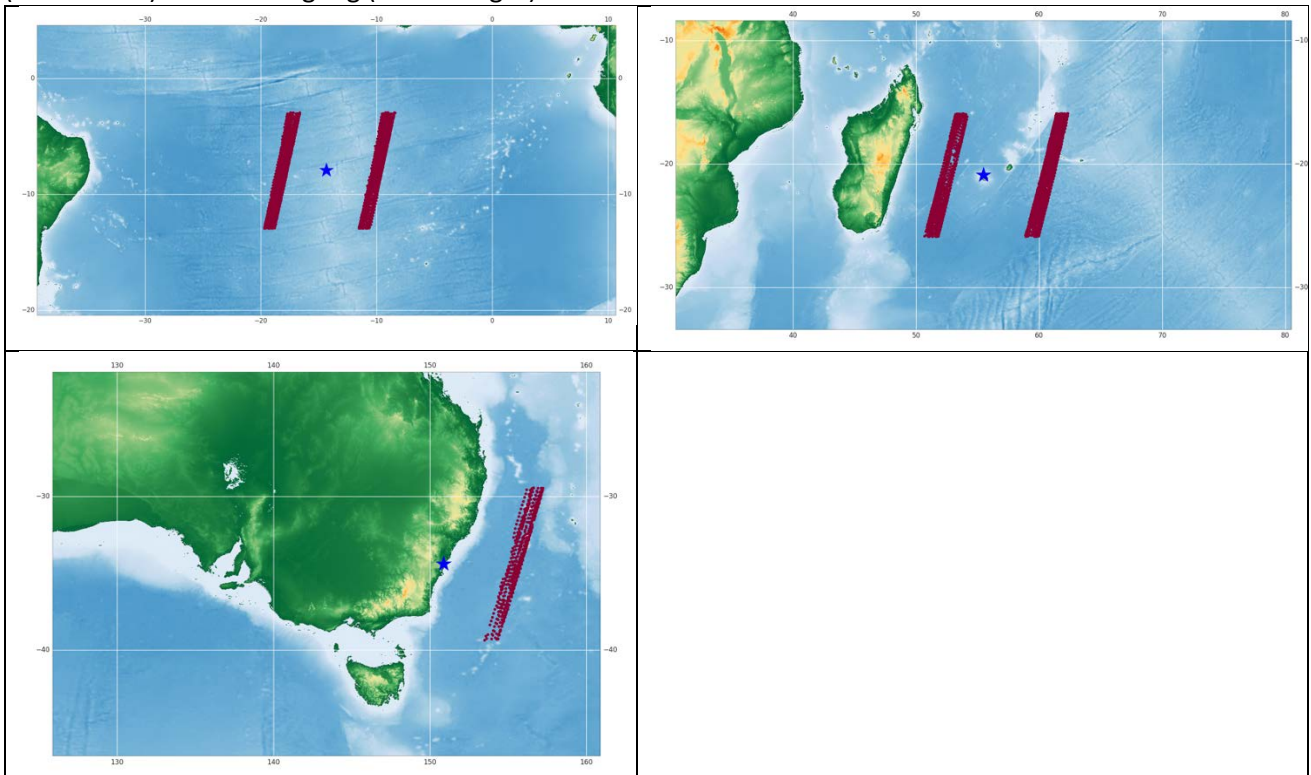


Figure 3: As Fig 1 but for sunglint soundings. Stations are Ascension (top left), Izana (top right), Reunion (bottom left) and Wollongong (bottom right).



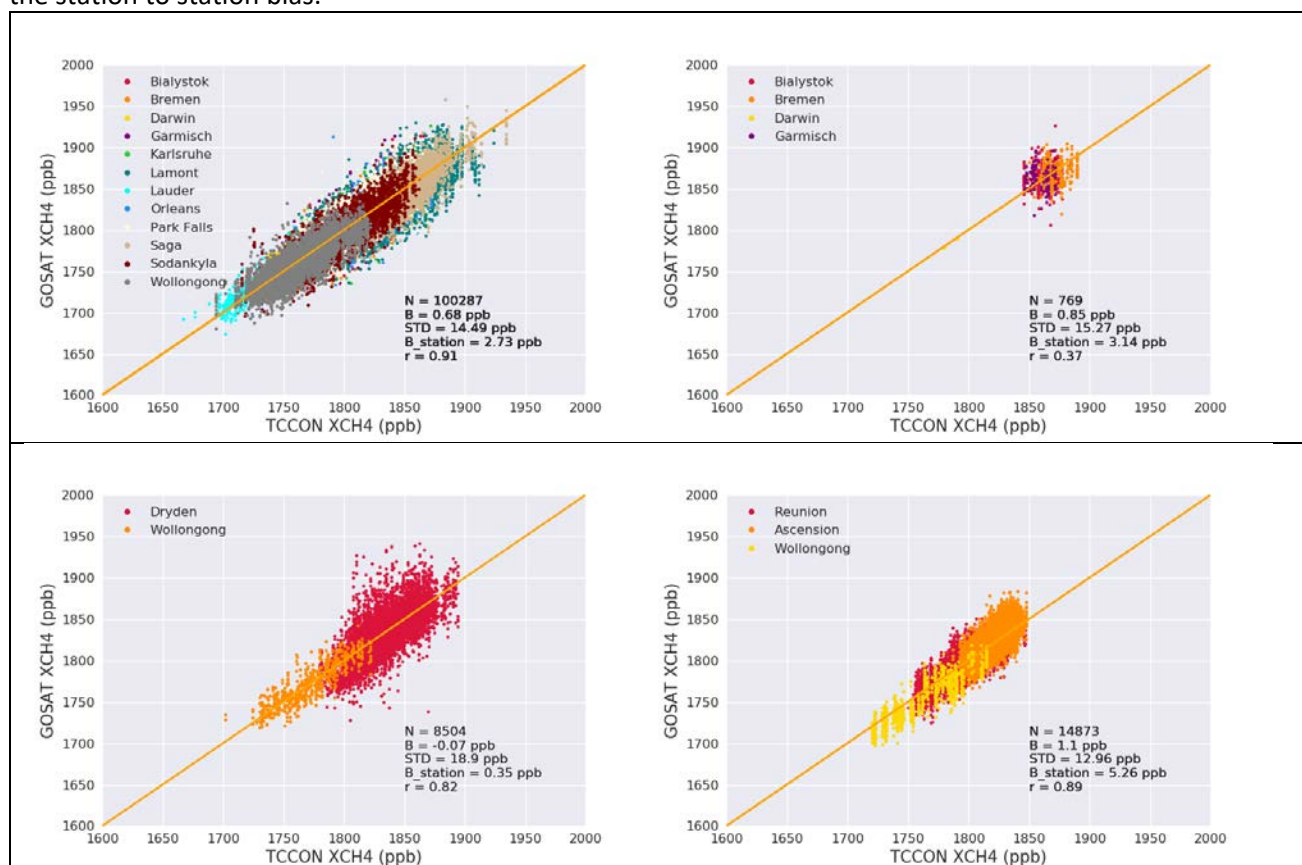


2. Validation Results

2.1 Product CH₄_GOS_SRPR

2.1.1 Validation

Figure 4: Validation of XCH₄ retrieved by GOSAT-RemoTeC with ground based TCCON measurements for gain H (Top left), gain H year 2020 only (top right), gain M (bottom left) and sunglint (bottom right) soundings. N(coloc) indicates the number of GOSAT-TCCON collocations, B indicates the bias between GOSAT and TCCON, and STD the standard deviation of the GOSAT TCCON difference (for individual measurements) and B_station the station to station bias.



The above figures all show a strong correlation of the retrieved (bias-corrected) XCH₄ with the TCCON XCH₄ ($r \sim 0.9$). This gives us confidence that our bias correction based on the retrieved albedo works correctly and takes out most of the bias. The 2020 only data shows a remaining bias of 0.85 ppb.

The figure below (Fig 5) shows in detail for each station the remaining bias and standard deviation for the co-located GOSAT soundings. Unlike for the CO₂_GOS_SRFP dataset, we do not include Izana here in the gain M validation, as its high altitude causes a large offset between measurements at the TCCON station and the Sahara desert.



In the case of gain H, the station to station standard deviation is 2.73 ppb. Saga also remains an outlier with a strong remaining negative bias, possibly due to inclusion of soundings in more polluted areas. Garmisch and Park Falls both show a positive offset, possibly due to the elevation of the TCCON stations (740 and 440 m respectively). Lamont clearly shows the most co-locations and dominates the total statistical comparison.

For gain M and sunglint we removed Darwin from the comparison as using the static spatial co-location criterion it only had limited co-located measurements.

Figure 5: The bias, standard deviation and # of measurements per station for gain H (top), gain M (middle) and sunglint (bottom) soundings for the period between the year 2009 and 2020.

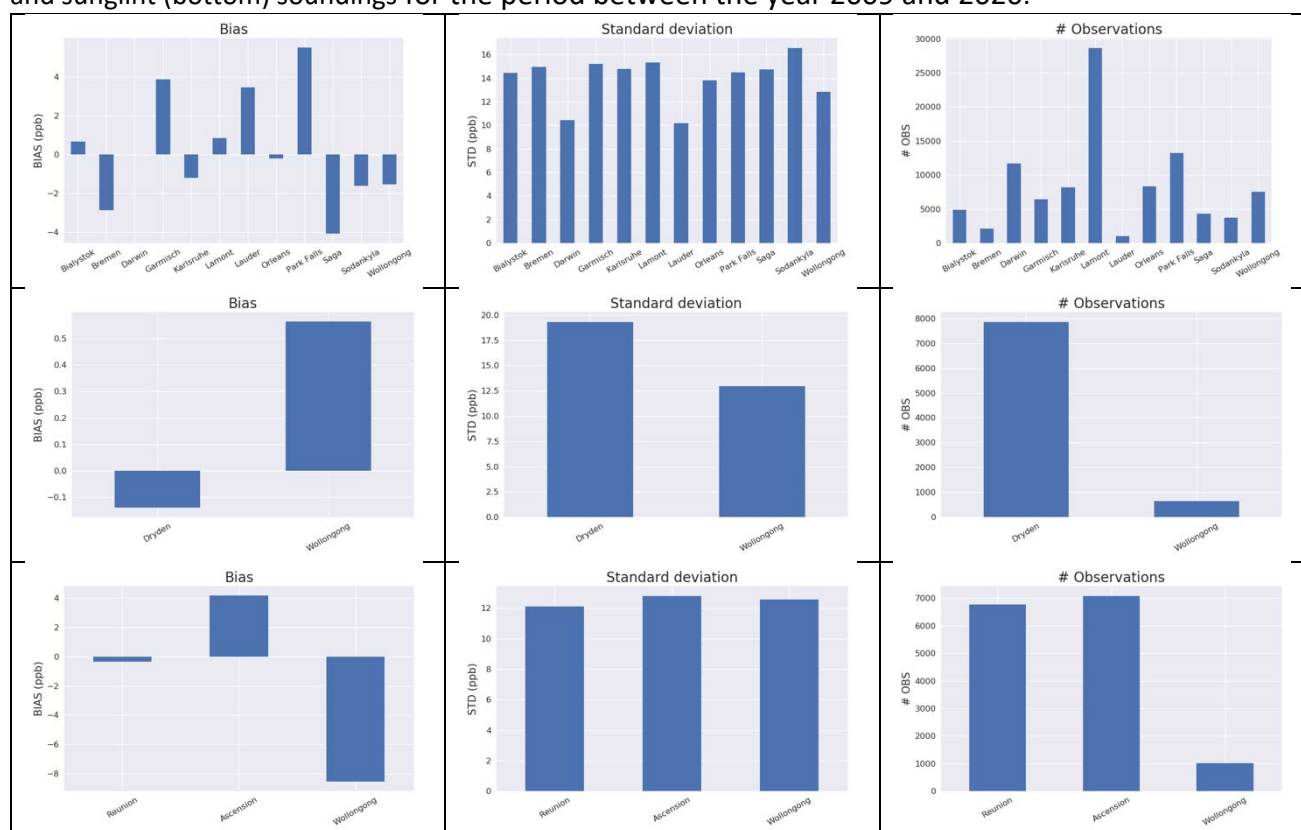
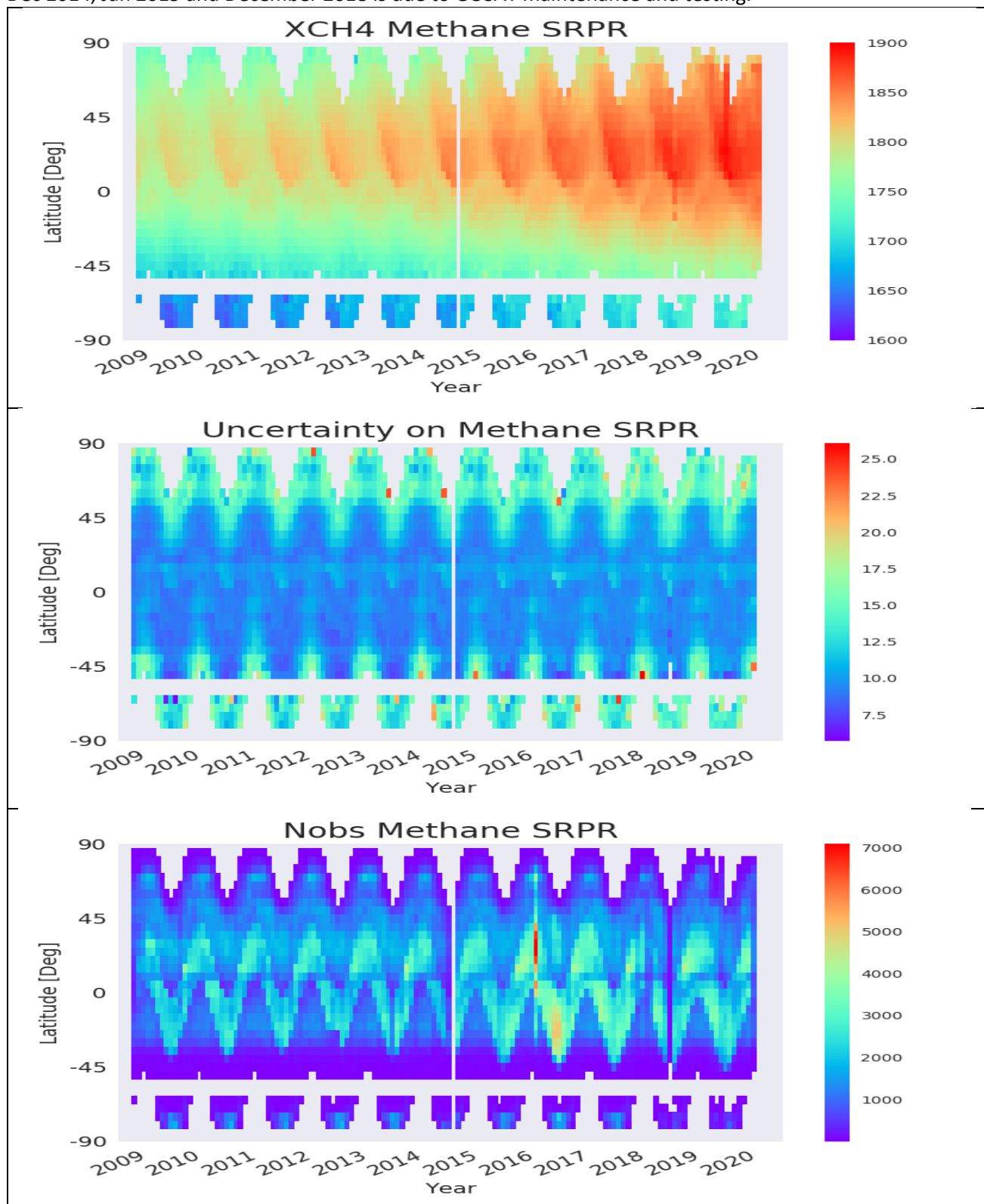




Figure 6: The CH₄_GOS_SRPR global dataset in slices of 10 degrees latitude as a function of time. The increase in XCH₄ concentrations during the last couple of years can clearly be seen. The gap in data coverage during Dec 2014, Jan 2015 and December 2018 is due to GOSAT maintenance and testing.





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 data products.

Fig. 7-11 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 7: Timeseries for the individual stations for gain H.

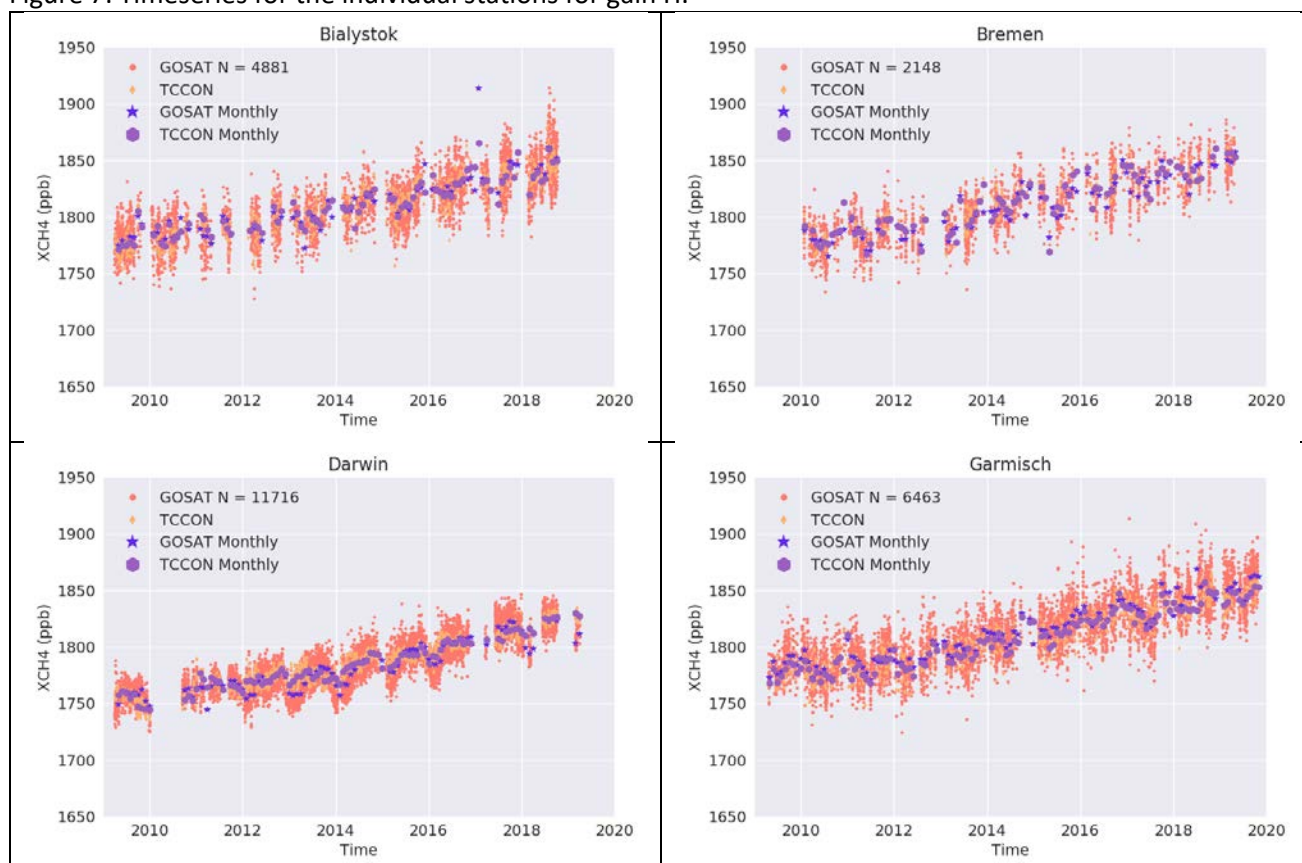




Figure 8: Timeseries for the individual stations for gain H (continued from Fig 7).

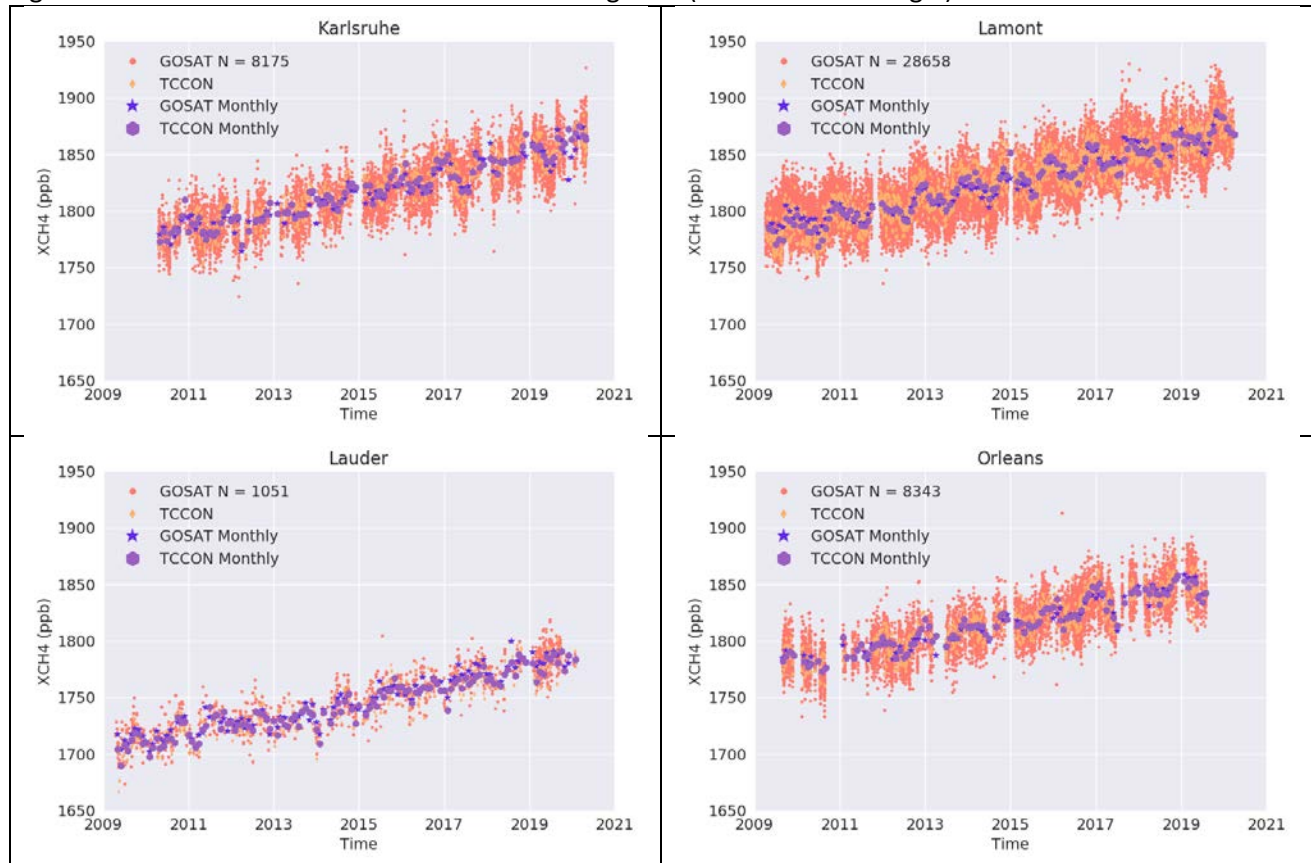




Figure 9: Timeseries for the individual stations for gain H (continued from Fig 7).

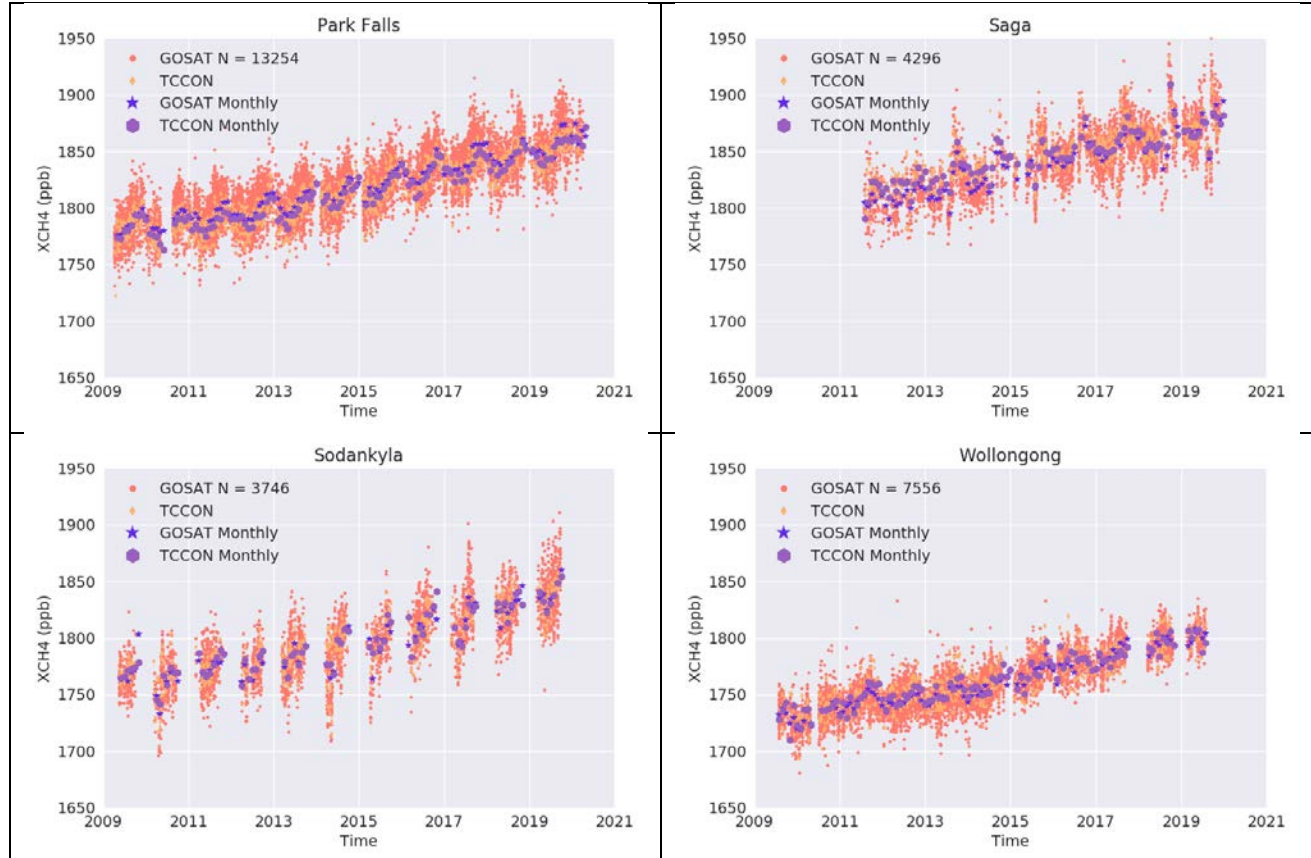




Figure 10: Timeseries for the individual stations for gain M.

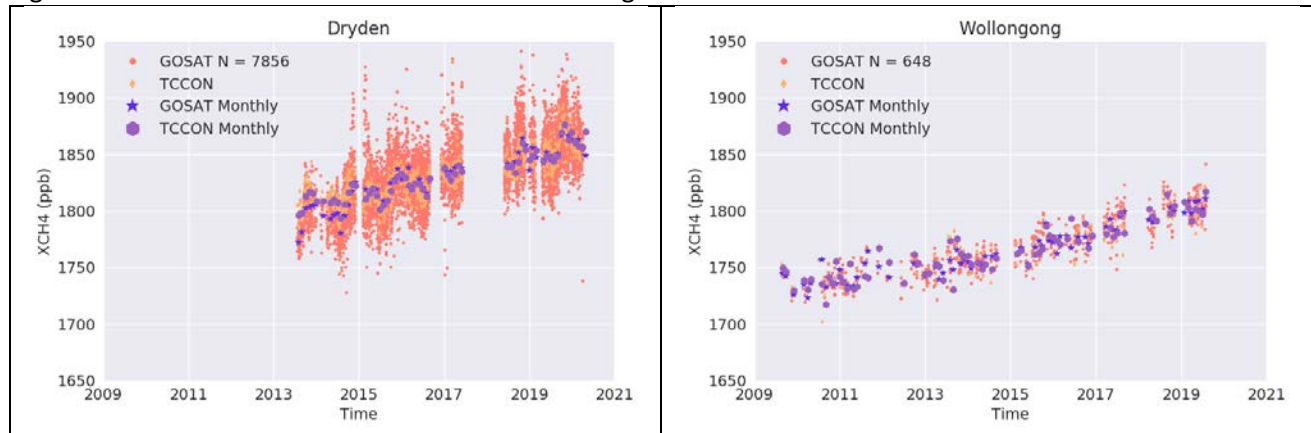
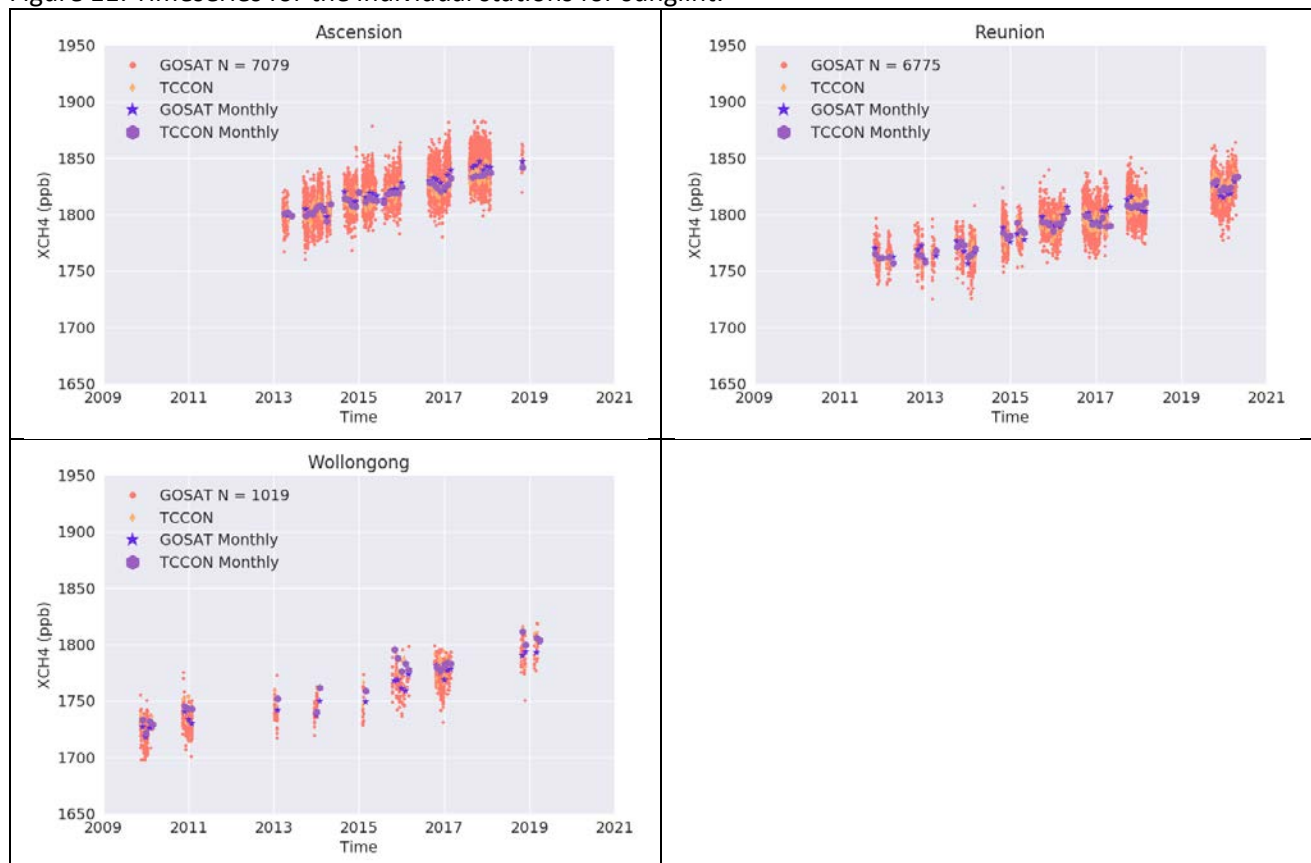


Figure 11: Timeseries for the individual stations for sunglint.





2.1.3 Validation summary

The validation results are summarized in the table below.

Table 2 - Product Quality Summary Table for product CH4_GOS_SRPR.

Product Quality Summary Table for Product: CH4_GOS_SRPR Level: 2, Version: 2.3.9, Time period covered: 06.2009 – 06.2020				
Parameter [unit]	Achieved performance	Requirement	TR	Comments
Single measurement precision (1-sigma) in [ppb]	14.49	< 34 (T) < 17 (B) < 9 (G)	-	-
Uncertainty ratio) in [-]: Ratio reported uncertainty to standard deviation of satellite-TCCON difference	1.26	-	-	No requirement but value close to unity expected for a high quality data product.
Mean bias [ppb]	0.68	-	-	No requirement but value close to zero expected for a high quality data product.
Accuracy: Relative systematic error [ppb]	Spatial – spatiotemporal: 2.73 – 5.26	< 10	Probability that accuracy TR is met: 87%	-
Stability: Linear bias trend [ppb/year]	-0.29 +/- 0.20 (1-sigma)	< 3	Probability that stability TR is met: 99%	-
Stability: Year-to-year bias variability [ppb/year]	7.83 +/- 2.42 (1-sigma)	< 3	-	-



3. Application(s) specific assessments

No application specific assessments have been carried out.

4. Compliance with user requirements

For the CH4_GOS_SRPR product we achieved 100% for TR's Accuracy and 100 % for TR's Stability



References

- Buchwitz et al., 2015:** Buchwitz, M., Reuter, M., Schneising, O., Boesch, H., Guerlet, S., Dils, B., Aben, I., Armante, R., Bergamaschi, P., Blumenstock, T., Bovensmann, H., Brunner, D., Buchmann, B., Burrows, J.P., Butz, A., Chédin, A., Chevallier, F., Crevoisier, C.D., Deutscher, N.M., Frankenberg, C., Hase, F., Hasekamp, O.P., Heymann, J., Kaminski, T., Laeng, A., Lichtenberg, G., De Mazière, M., Noël, S., Notholt, J., Orphal, J., Popp, C., Parker, R., Scholze, M., Sussmann, R., Stiller, G.P., Warneke, T., Zehner, C., Bril, A., Crisp, D., Griffith, D.W.T., Kuze, A., O'Dell, C., Oshchepkov, S., Sherlock, V., Suto, H., Wennberg, P., Wunch, D., Yokota, T., Yoshida, Y., 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 Sens. Environ.* 162:344–362, <http://dx.doi.org/10.1016/j.rse.2013.04.024>, 2015.
- Buchwitz et al., 2016:** Buchwitz, M., Reuter, M., Schneising, O., Hewson, W., Detmers, R. G., Boesch, H., Hasekamp, O. P., Aben, I., Bovensmann, H., Burrows, J. P., Butz, A., Chevallier, F., Dils, B., Frankenberg, C., Heymann, J., Lichtenberg, G., De Mazière, M., Notholt, J., Parker, R., Warneke, T., Zehner, C., Griffith, D. W. T., Deutscher, N. M., Kuze, A., Suto, H., and Wunch, D.: Global satellite observations of column-averaged carbon dioxide and methane: The GHG-CCI XCO₂ and XCH₄ CRDP3 data, *Remote Sensing of Environment* (in press), Special Issue on Essential Climate Variables, DOI: 10.1016/j.rse.2016.12.027, (link: <http://dx.doi.org/10.1016/j.rse.2016.12.027>), 2016.
- Buchwitz et al., 2017:** ESA Climate Change Initiative (CCI) Product Validation and Intercomparison Report (PVIR) for the Essential Climate Variable (ECV) Greenhouse Gases (GHG) for data set Climate Research Data Package No. 4 (CRDP#4), Version 5.0, 9. Feb. 2017, link: http://www.esa-ghg-cci.org/?q=webfm_send/352, 2017.
- Buchwitz et al., 2017a:** Buchwitz, M.; Reuter, M.; Aben, I.; Boesch, H.; Butz, A.; Detmers, R.G.; Frankenberg, C.; Hasekamp, O.P.; Parker, R.; Schneising, O.; Somkuti, P., ESA Greenhouse Gases Climate Change Initiative (GHG-CCI): Merged SCIAMACHY and GOSAT Level 3 gridded atmospheric column-average methane (XCH₄) product in Obs4MIPs format version 2 (CRDP#4), Technical Note, link: http://www.esa-ghg-cci.org/?q=webfm_send/349, pp. 11, 1 February 2017, 2017.
- Butz et al., 2011:** Butz, A., Guerlet, S., Hasekamp, O., et al., Toward accurate CO₂ and CH₄ observations from GOSAT, *Geophys. Res. Lett.*, doi:10.1029/2011GL047888, 2011.
- Butz et al., 2012:** Butz, A., Galli, A., Hasekamp, O., Landgraf, J., Tol, P., and Aben, I.: Remote Sensing of Environment, TROPOMI aboard Sentinel-5 Precursor : Prospective performance of CH₄ retrievals for aerosol and cirrus loaded atmospheres, 120, 267-276, doi:10.1016/j.rse.2011.05.030, 2012.
- Detmers et al., 2015:** Detmers, R. G., O. Hasekamp, I. Aben, S. Houweling, T. T. van Leeuwen, A. Butz, J. Landgraf, P. Koehler, L. Guanter, and B. Poulter, [Anomalous carbon uptake in Australia as seen by GOSAT](#), *Geophys. Res. Lett.*, 42, doi:10.1002/2015GL065161, 2015.
- ESA-CCI-GHG-URDv2.1:** Chevallier, F., et al., User Requirements Document (URD), ESA Climate Change Initiative (CCI) GHG-CCI project, Version 2.1, 19 Oct 2016, link: http://www.esa-ghg-cci.org/?q=webfm_send/344, 2016.



- Kuze et al., 2009:** Kuze, A., Suto, H., Nakajima, M., and Hamazaki, T. (2009), Thermal and near infrared sensor for carbon observation Fourier-transform spectrometer on the Greenhouse Gases Observing Satellite for greenhouse gases monitoring, *Appl. Opt.*, 48, 6716–6733, 2009.
- Kuze et al., 2016:** Kuze, A., Suto, H., Shiomi, K., Kawakami, S., Tanaka, M., Ueda, Y., Deguchi, A., Yoshida, J., Yamamoto, Y., Kataoka, F., Taylor, T. E., and Buijs, H. L.: Update on GOSAT TANSO-FTS performance, operations, and data products after more than 6 years in space, *Atmos. Meas. Tech.*, 9, 2445–2461, doi:10.5194/amt-9-2445-2016, 2016.
- Schepers et al., 2012:** Schepers, D., Guerlet, S., Butz, A., Landgraf, J., Frankenberg, C., Hasekamp, O., Blavier, J.-F., Deutscher, N. M., Griffith, D. W. T., Hase, F., Kyro, E., Morino, I., Sherlock, V., Sussmann, R., Aben, I. (2012), 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.
- TRD GHG, 2017:** Buchwitz, M., Aben, I., Anand, J., Armante, R., Boesch, H., Crevoisier, C., Detmers, R. G., Hasekamp, O. P., Reuter, M., Schneising-Weigel, O., Target Requirement Document, Copernicus Climate Change Service (C3S) project on satellite-derived Essential Climate Variable (ECV) Greenhouse Gases (CO₂ and CH₄) data products (project C3S_312a_Lot6), Version 1, 28-March-2017, pp. 52, 2017.
- TRD GAD GHG, 2020:** Buchwitz, M., Aben, I., Armante, R., Boesch, H., Crevoisier, C., Hasekamp, O. P., Wu, L., Reuter, M., Schneising-Weigel, O., Target Requirement and Gap Analysis Document, Copernicus Climate Change Service (C3S) project on satellite-derived Essential Climate Variable (ECV) Greenhouse Gases (CO₂ and CH₄) data products (project C3S_312b_Lot2), Version 2.11, 9-April-2020, pp. 80, 2020.
- 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.
- Yokota et al., 2009:** Yokota, T., Y. Yoshida, N. Eguchi, Y. Ota, T. Tanaka, H. Watanabe, and S. Maksyutov (2009), Global concentrations of CO₂ and CH₄ retrieved from GOSAT: First preliminary results, *SOLA*, 5, 160–163.
- Yoshida et al., 2010:** Yoshida, Y., Y. Ota, N. Eguchi, N. Kikuchi, K. Nobuta, H. Tran, I. Morino, and T. Yokota (2010), Retrieval algorithm for CO₂ and CH₄ column abundances from short-wavelength infrared spectral observations by the greenhouse gases observing satellite, *Atmospheric Measurement Techniques Discussions*, 3(6), 4791–4833, doi:10.5194/amtd-3-4791-2010.

Copernicus Climate Change Service

ECMWF - Shinfield Park, Reading RG2 9AX, UK

Contact: info@copernicus-climate.eu

climate.copernicus.eu

copernicus.eu

ecmwf.int