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Product Quality Assessment Report (PQAR) – ANNEX B for products CO2_GOS_SRFP (v2.3.8, 2009-2017) & CH4_GOS_SRFP (v2.3.8, 2009-2017)

C3S_312a_Lot6_IUP-UB – Greenhouse Gases

Issued by: R. G. Detmers, SRON, The Netherlands

Date: 04/10/2018

Ref: C3S_D312a_Lot6.3.1.7-v2_PQAR_ANNEX-B_v2.0

Official reference number service contract: 2016/C3S_312a_Lot6_IUP-UB/SC1

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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

Related documents

Reference ID	Document
D1	Main PQAR: Buchwitz, M., et al., Product Quality Assessment Report (PQAR) – Main document, C3S project C3S_312a_Lot6_IUP-UB – Greenhouse Gases, v2.0, 2018. *(this document is an ANNEX to the Main PQAR)*

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/) component as covered by project C3S_312a_Lot6 led by University of Bremen, Germany.

Within project C3S_312a_Lot6 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 C3S_312a_Lot 6 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 C3S products CO2_GOS_SRFP and CH4_GOS_SRFP.

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

Executive summary

This report summarizes the performance of the RemoTeC CO2_GOS_SRFP and CH4_GOS_SRFP retrievals. In general, we find very good agreement with TCCON data for all three modes (gain H, gain M and sunglint) for both products. All have a very high degree of correlation with TCCON (R~0.9).
For the CO2_GOS_SRFP product the station to station bias is 0.43 ppm and a standard deviation of around 1.92 ppm is observed for most TCCON stations. For the CH4_GOS_SRFP product the station to station bias is 3.45 ppb and a standard deviation of around 14.33 ppb is observed for most TCCON stations. We also checked the stability of the bias over time for both products as the GOSAT time series now spans a period of 8.5 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 (100 % chance TR is met) for accuracy and stability for the CH4_GOS_SRFP product, while for CO2_GOS_SRFP we achieved a 54 % chance that the TR is met for accuracy and a 100 % chance that the TR is met for stability.

1. Product validation methodology

Validation of the CH4_GOS_SRFP and CO2_GOS_SRFP products is performed by comparison a selection of ground-based FTS TCCON stations. These provide total column XCH4 and XCO2 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

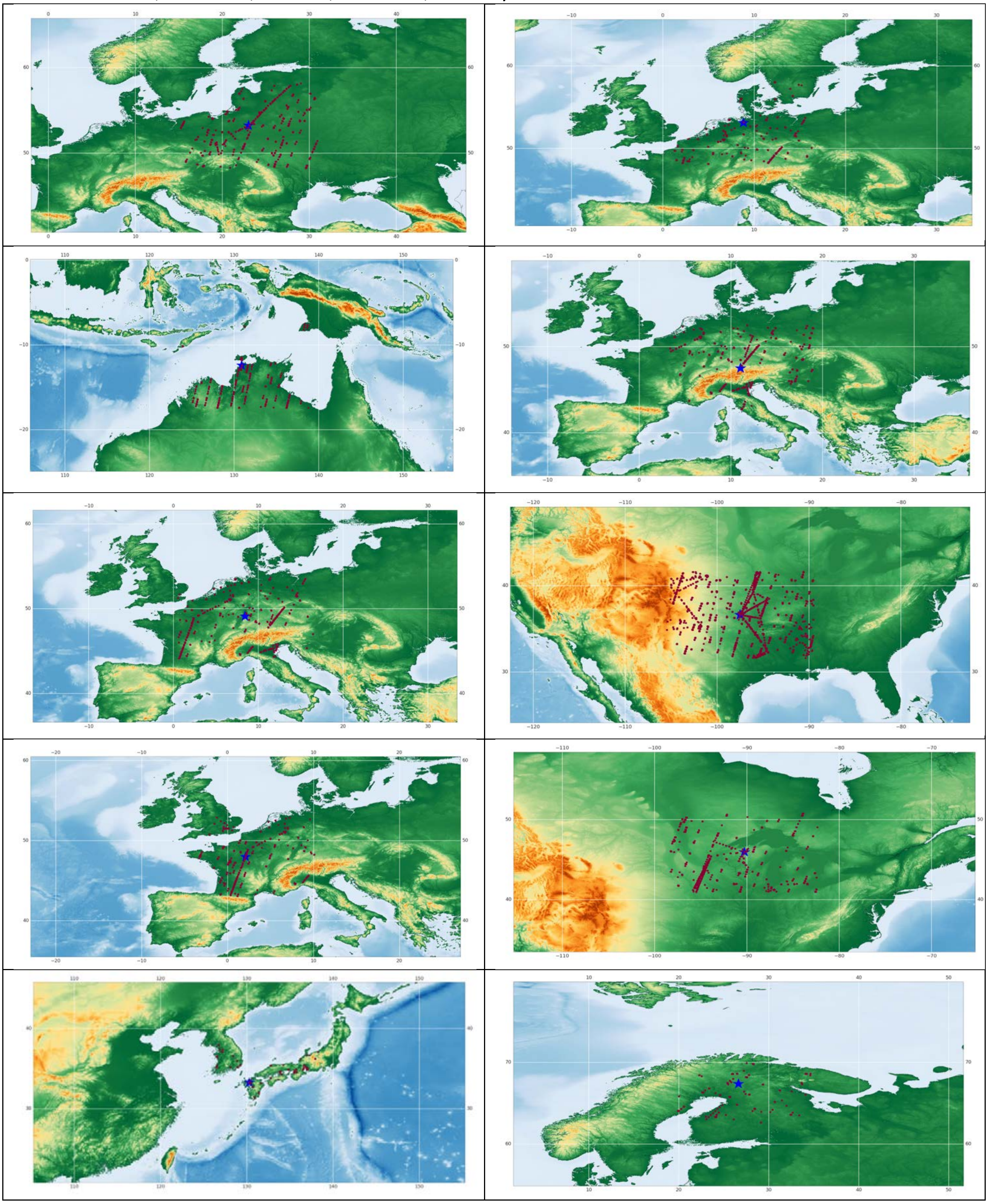
We co-locate the GOSAT soundings with the TCCON measurements using the following criteria:

- 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 2017 were not yet available. We therefore decided to use a box filter instead as we did want to include 2017 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 soundings for the gain H, gain M and sunglint stations respectively.

Figure 1: GOSAT co-located 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.



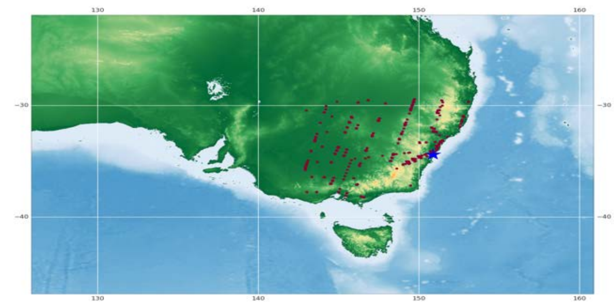


Figure 2: As Fig 1 but for gain M soundings. Stations are Dryden (top left), Izana (top right) and Wollongong (bottom left).

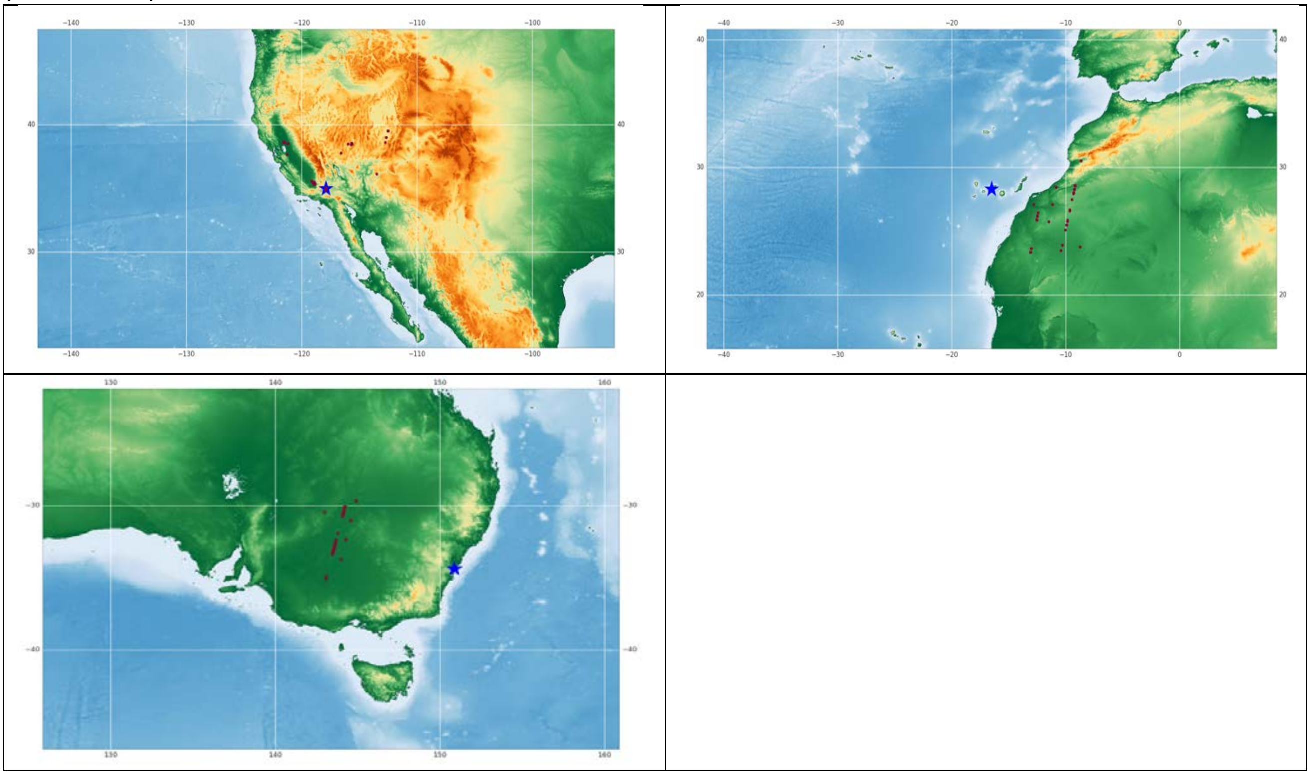
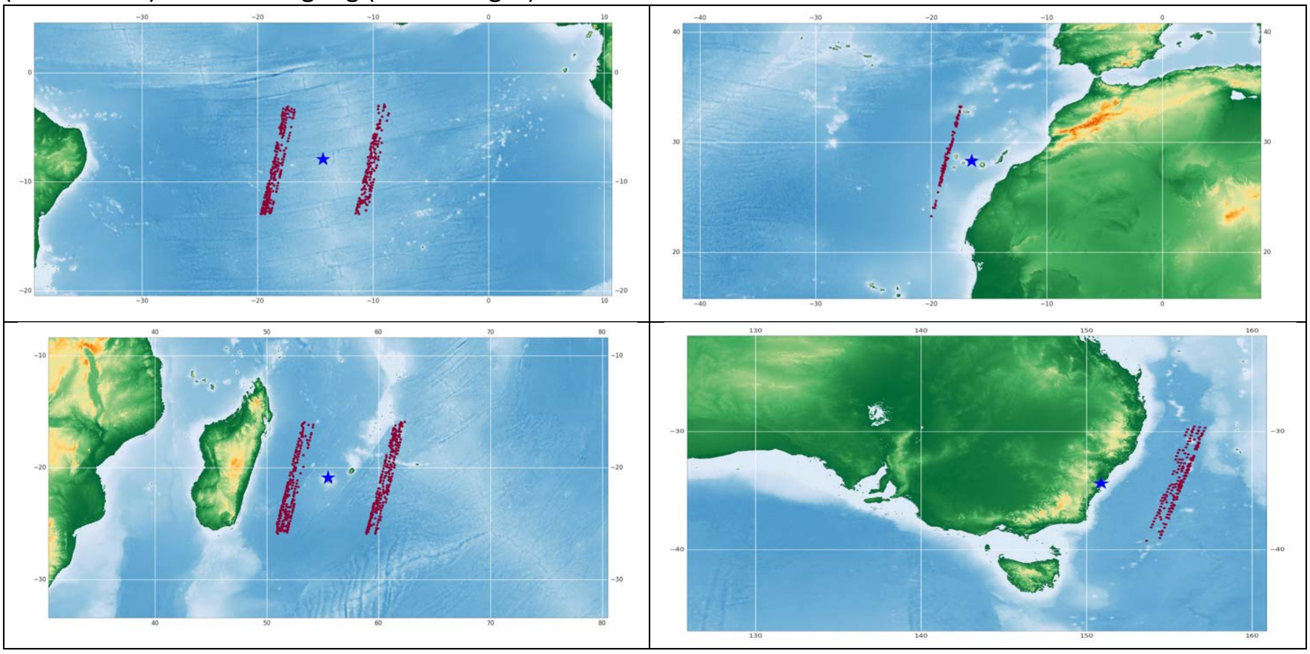


Figure 3: As Fig 1 but for sunglint soundings. Stations are Ascension (top left), Izana (top right), Reunion (bottom left) and Wollongong (bottom right).

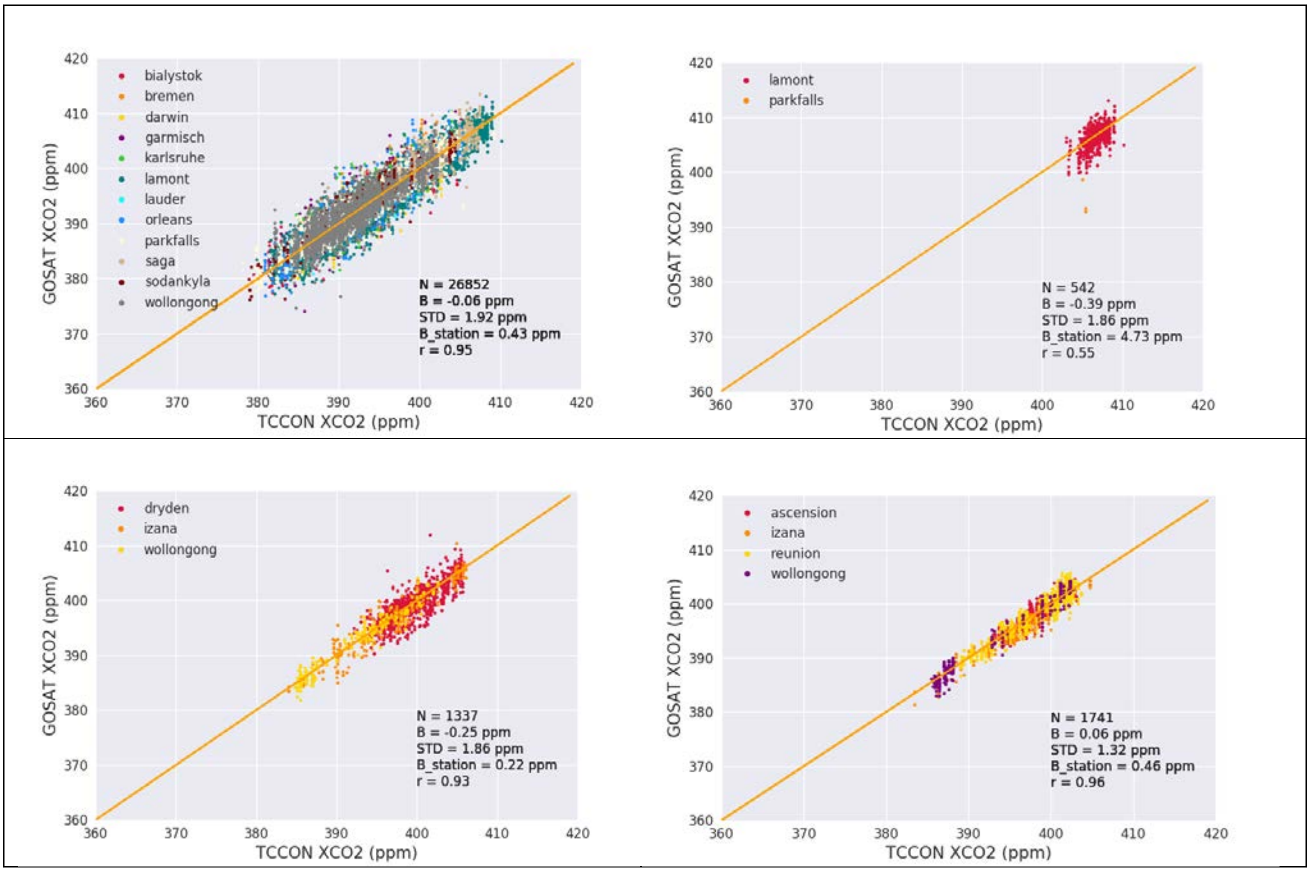


2. Validation Results

2.1 Product CO2_GOS_SRFP

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 2017 only (top right), gain M (bottom left) and sunglint (bottom right) soundings. N(coloc) indicates the number of GOSAT-TCCON colocations, 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) XCO2 with the TCCON XCO2 (r ~ 0.9). 2017 shows a smaller correlation but that is due to the limited range of XCO2 values covered in 2017 compared to the whole timeseries. This gives us confidence that our bias correction based on the retrieved albedo works correctly and takes out most of the bias.

The figure below (Fig 5) shows in detail for each station the remaining bias and standard deviation for the co-located GOSAT soundings. We include Izana in the gain M and sunglint validation to improve the otherwise limited gain M validation.

In the case of gain H, the station to station standard deviation is 0.32 ppm. Lamont shows a small negative remaining bias, while Sodankyla has a large positive remaining bias of almost 1 ppm. For

gain M and sunglint, Izana shows a negative bias. 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 4 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.

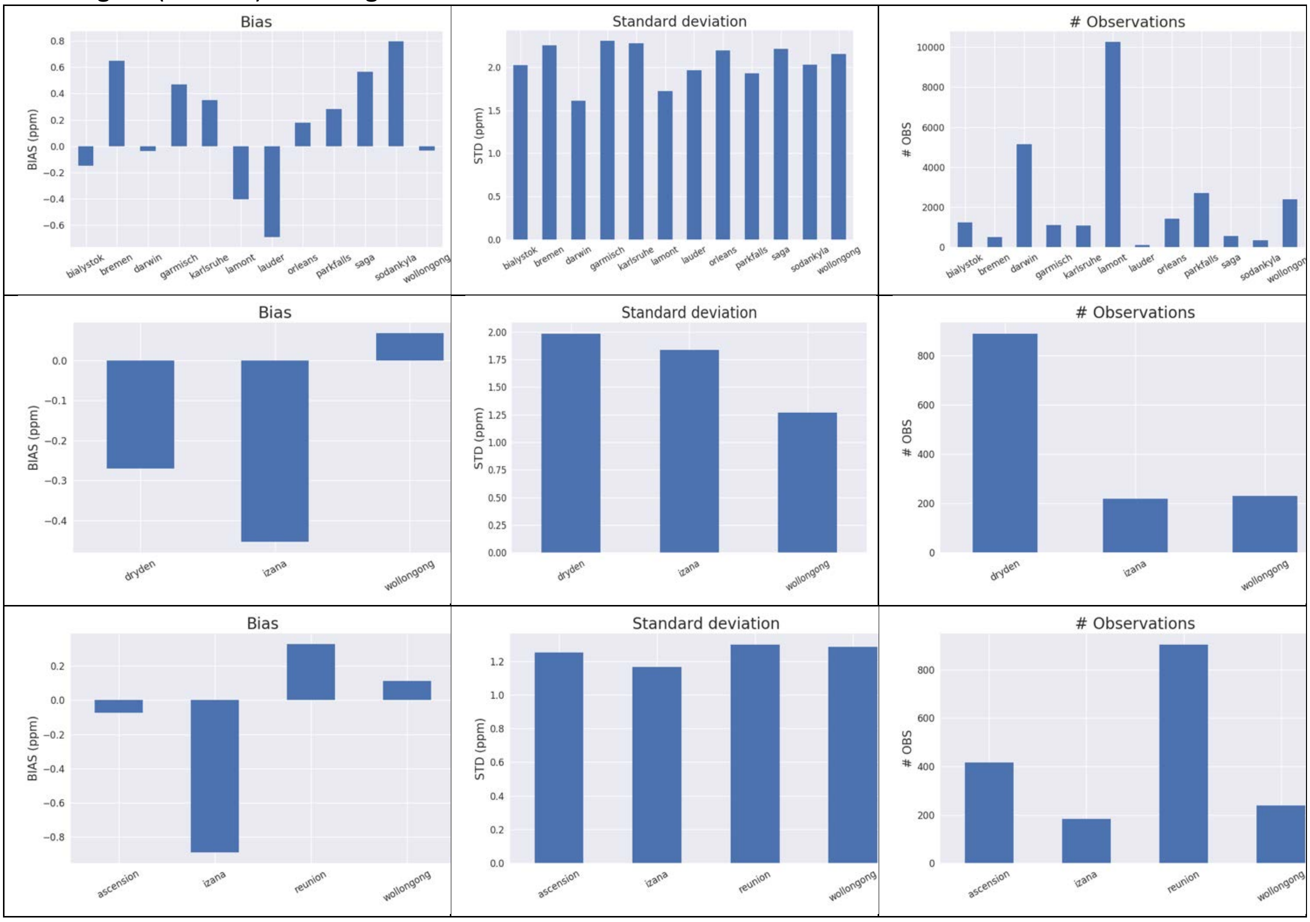
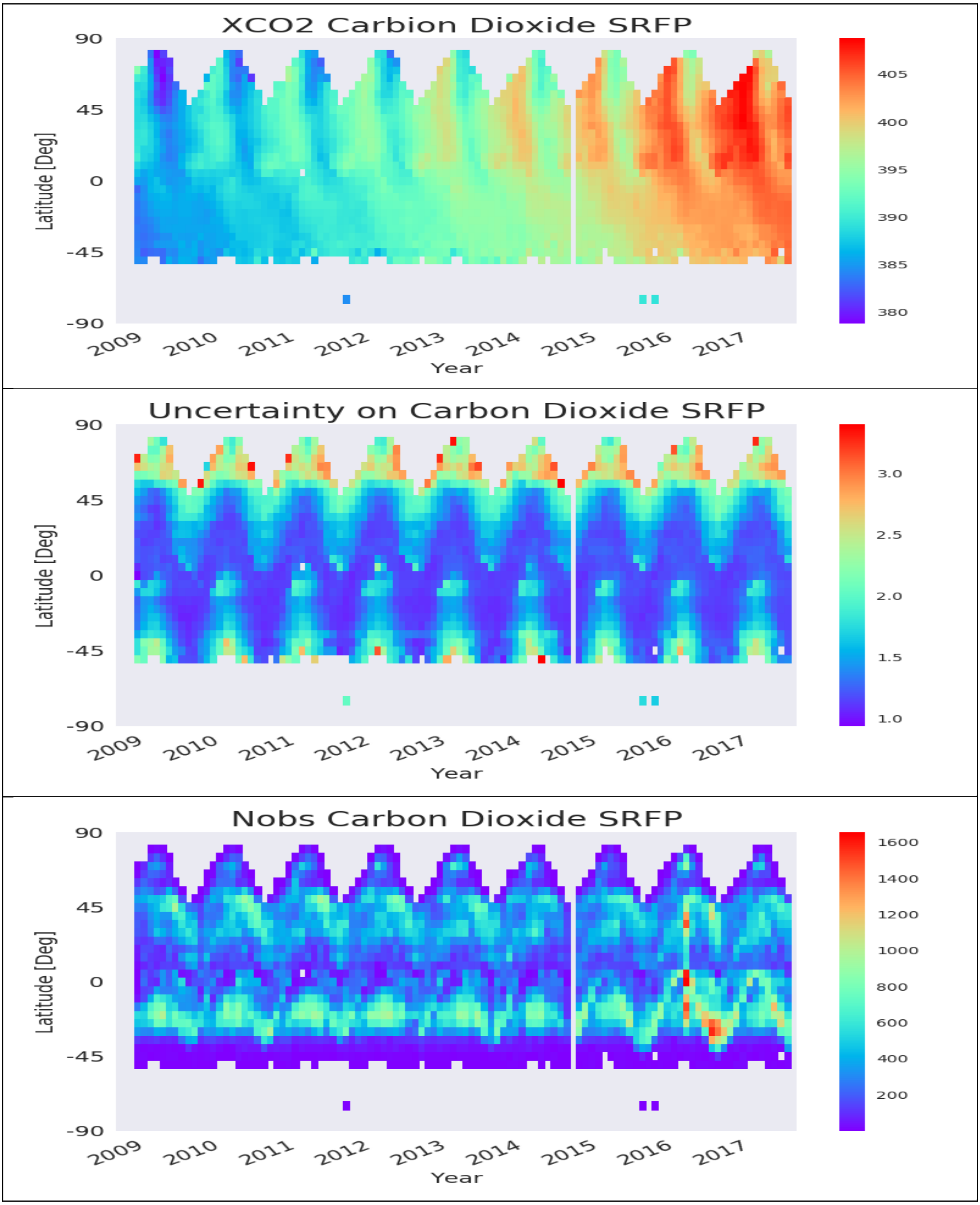


Figure 6: The CO2_GOS_SRFP global dataset in slices of 10 degrees latitude as a function of time. The yearly increase in XCO2 concentrations can clearly be seen. The gap in data coverage during Dec 2014 and Jan 2015 is due to GOSAT maintenance and testing.


XCO2 Carbion Dioxide SRFP
Latitude [Deg]
90
45
0
-45
-90
2009
2010
2011
2012
2013
2014
2015
2016
2017
Year
405
400
395
390
385
380
Uncertainty on Carbon Dioxide SRFP
Latitude [Deg]
90
45
0
-45
-90
2009
2010
2011
2012
2013
2014
2015
2016
2017
Year
3.0
2.5
2.0
1.5
1.0
Nobs Carbon Dioxide SRFP
Latitude [Deg]
90
45
0
-45
-90
2009
2010
2011
2012
2013
2014
2015
2016
2017
Year
1600
1400
1200
1000
800
600
400
200

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 timeseries 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 for CO2_GOS_SRFP.

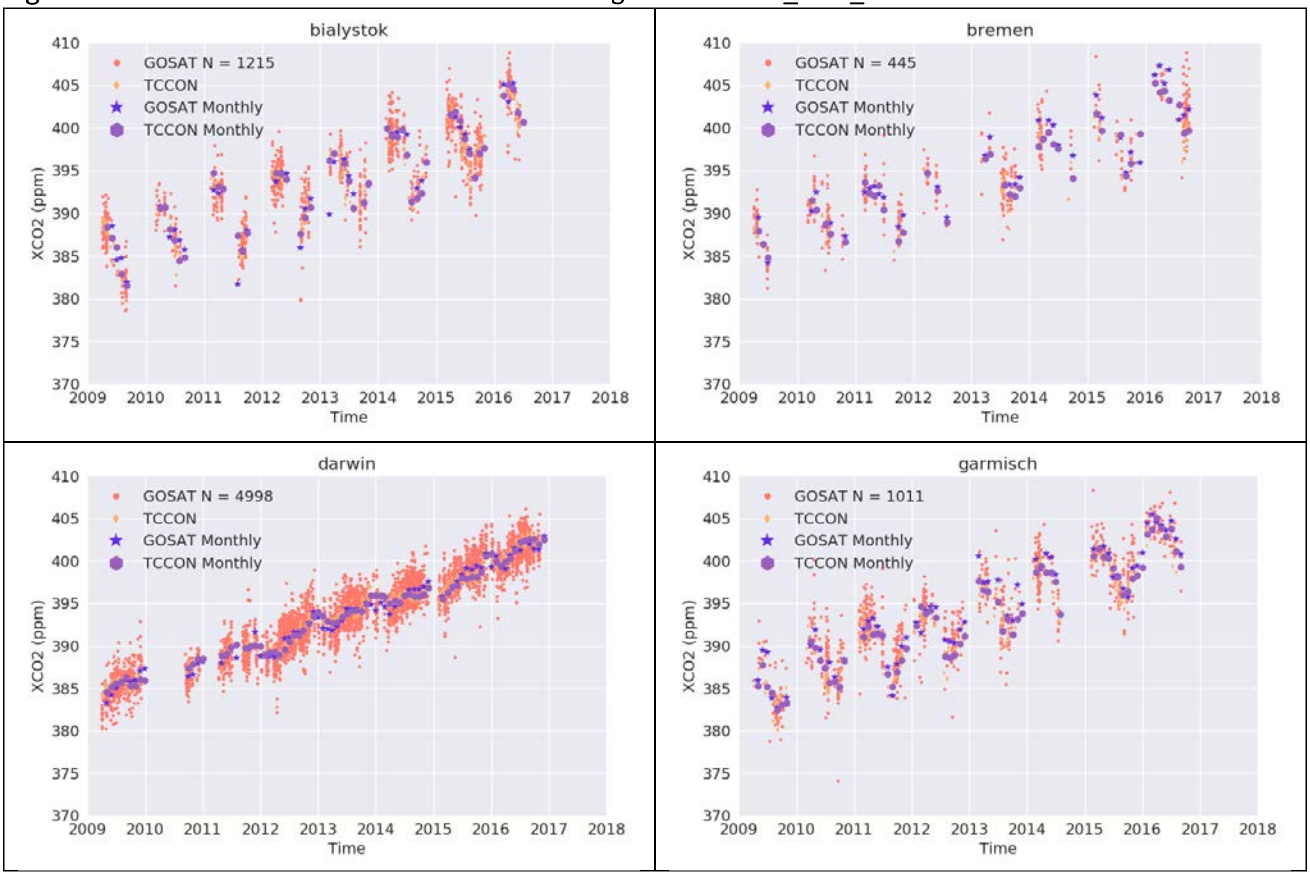


Figure 8: Timeseries for the individual stations for gain H for CO2_GOS_SRFP (continued from Fig 7).

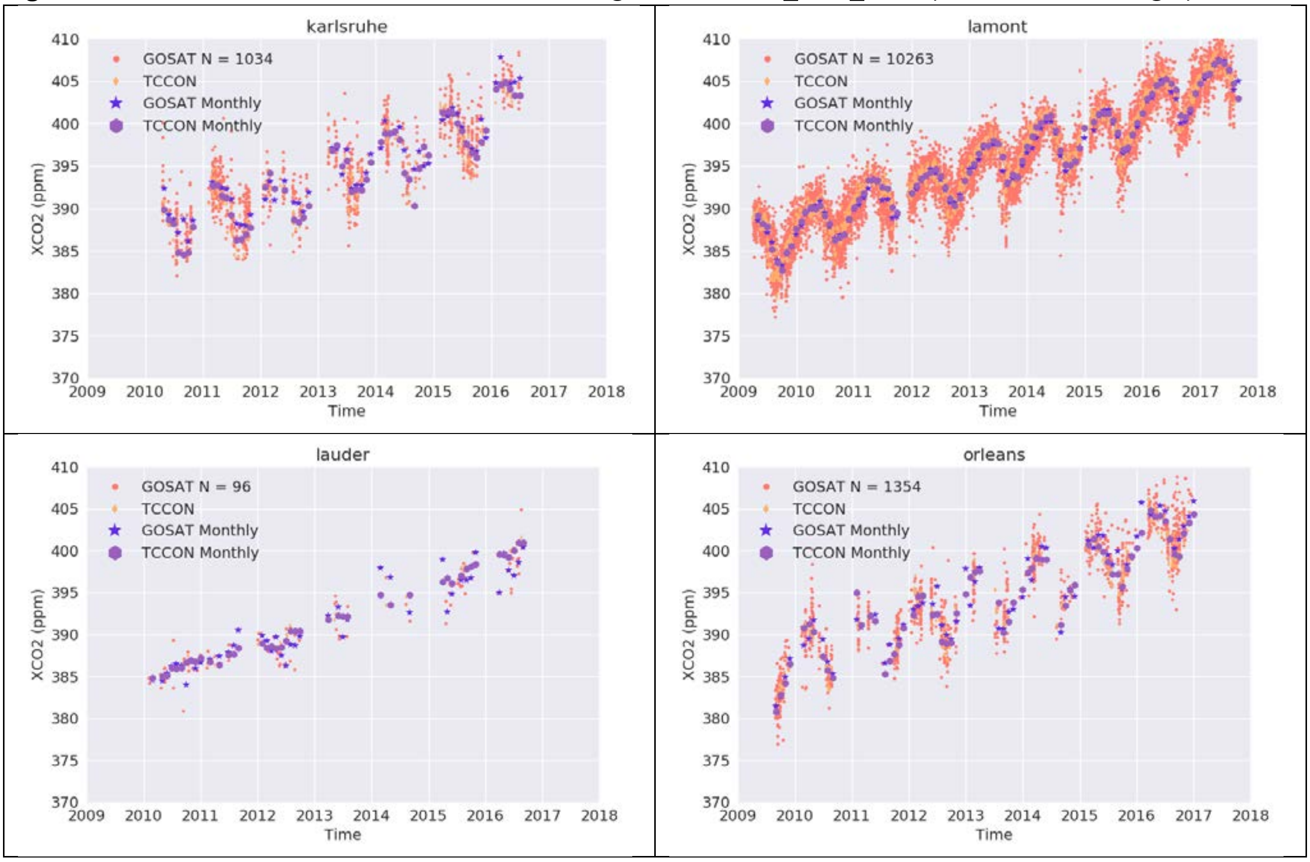
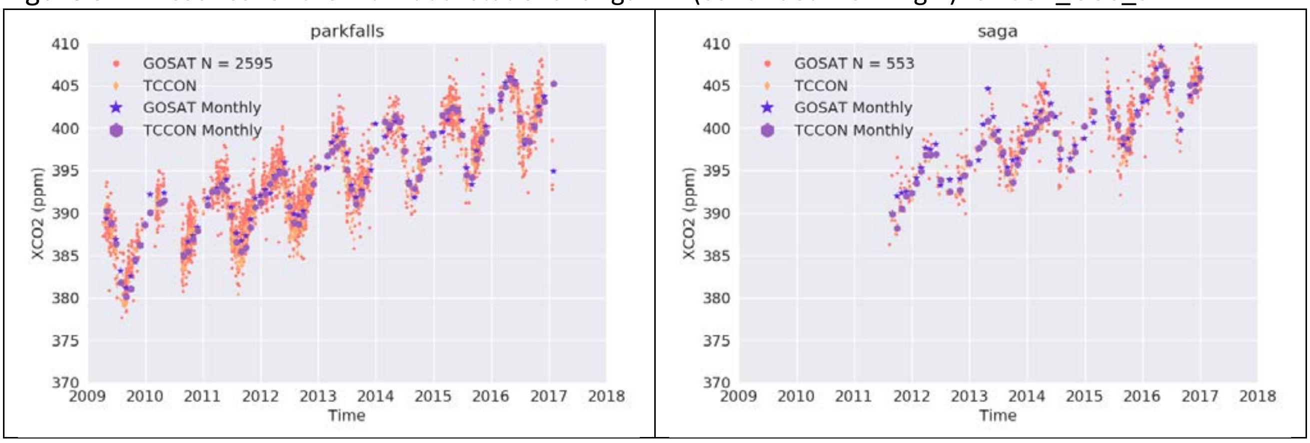


Figure 9: Timeseries for the individual stations for gain H (continued from Fig 7) for CO2_GOS_SRFP.



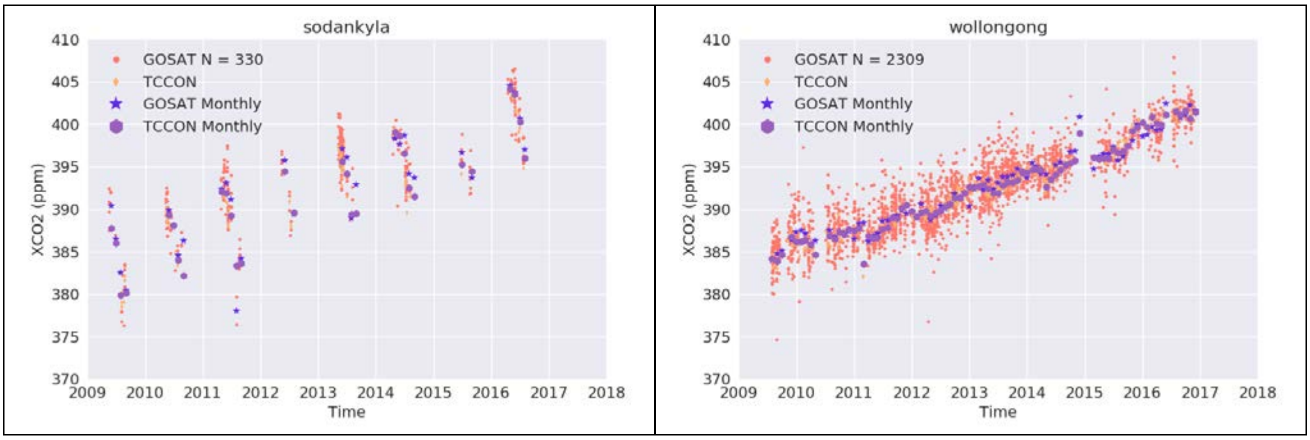


Figure 10: Timeseries for the individual stations for gain M for CO2_GOS_SRFP.

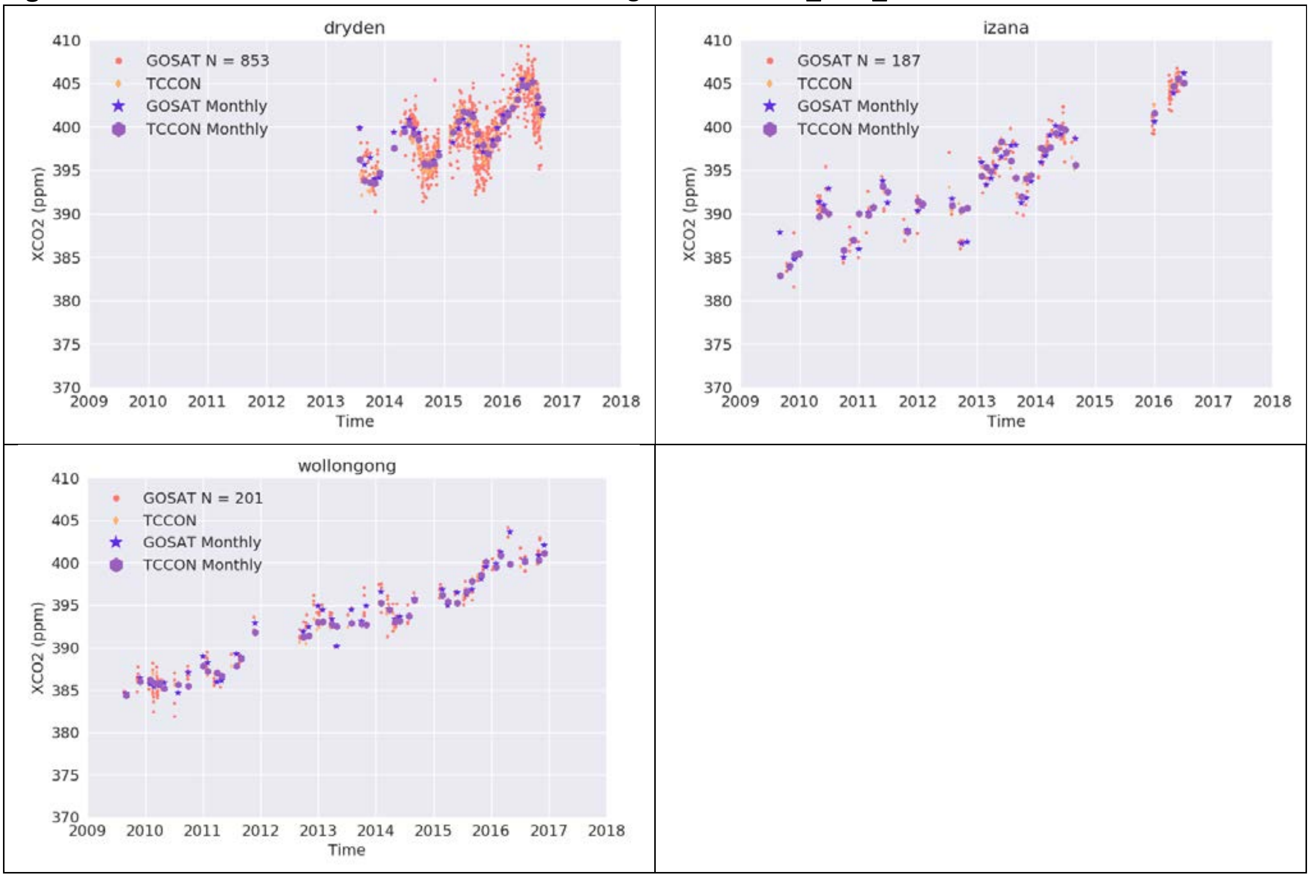
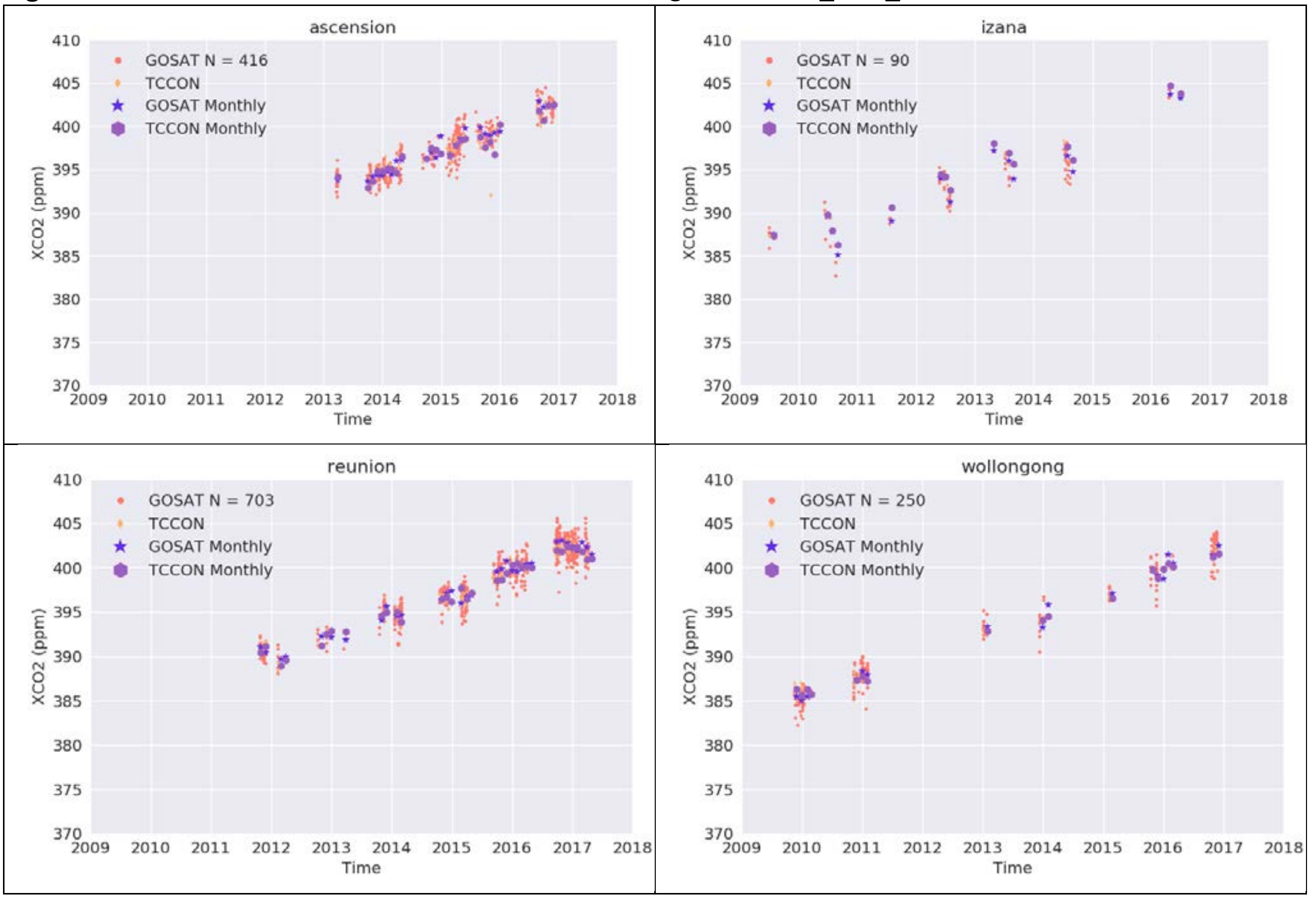


Figure 11: Timeseries for the individual stations for sunglint for CO2_GOS_SRFP.



2.1.3 Validation summary

The validation results are summarized in the table below.

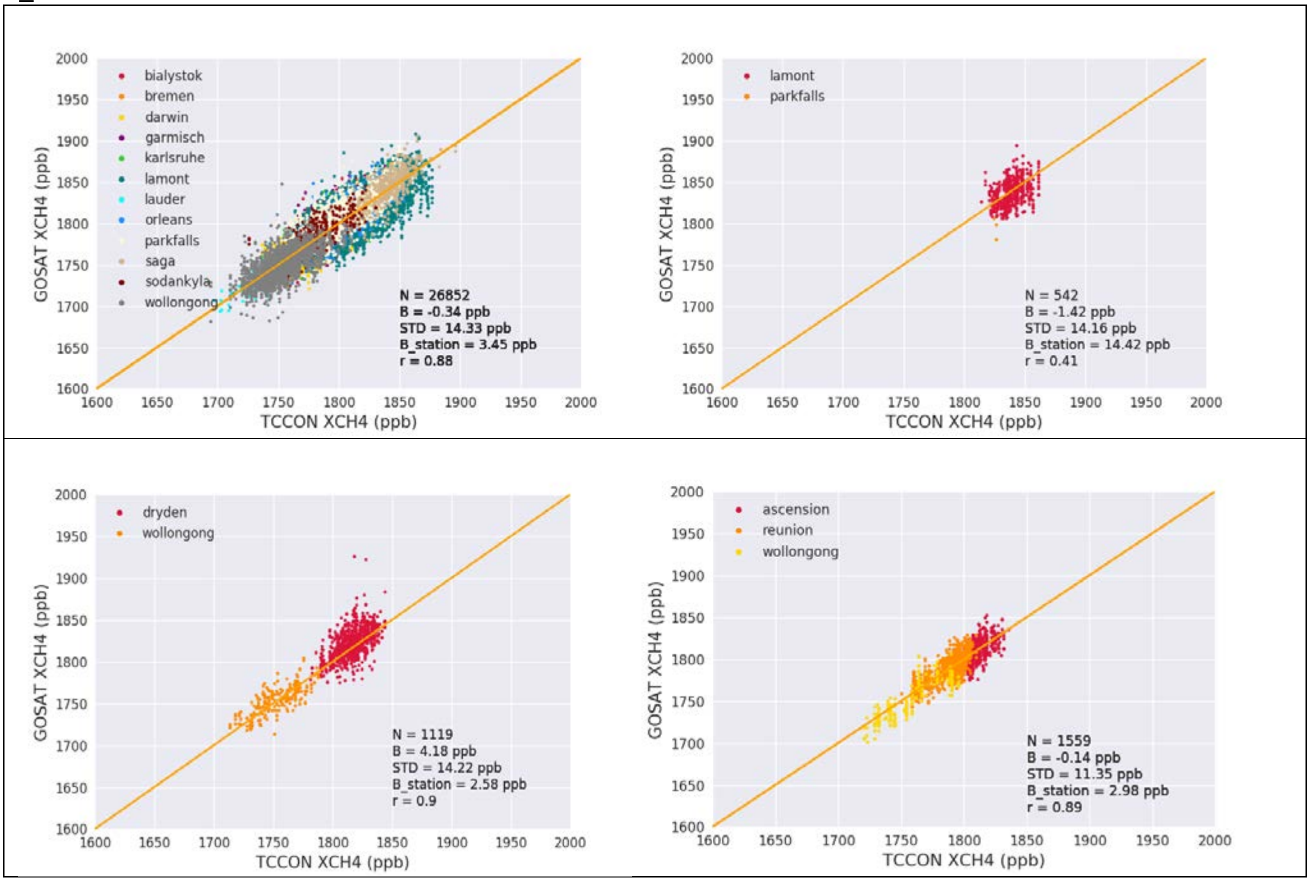
Table 2 - Product Quality Summary Table for product CO2_GOS_SRFP.

Product Quality Summary Table for Product: CO2_GOS_SRFP Level: 2, Version: 2.3.8, Time period covered: 6.2009 – 12.2017				
Parameter [unit]	Achieved performance	Requirement	TR	Comments
Single measurement precision (1-sigma) in [ppm]	1.92	< 8 (T) < 3 (B) < 1 (G)	-	-
Uncertainty ratio) in [-]: Ratio reported uncertainty to standard deviation of satellite-TCCON difference	1.10	-	-	No requirement but value close to unity expected for a high quality data product.
Mean bias [ppm]	-0.06	-	-	No requirement but value close to zero expected for a high quality data product.
Accuracy: Relative systematic error [ppm]	Spatial – spatiotemporal: 0.43-0.56	< 0.5	Probability that accuracy TR is met: 54 %	-
Stability: Drift [ppm/year]	-0.03 +/- 0.01 (1-sigma)	< 0.5	Probability that stability TR is met: 100 %	-
Stability: Year-to-year bias variability [ppm/year]	0.36 +/- 0.10 (1-sigma)	< 0.5	-	-

2.2 Product CH4_GOS_SRFP

2.2.1 Validation

Figure 12: Validation of XCH4 retrieved by GOSAT-RemoTeC with ground based TCCON measurements for gain H (Top left),gain H year 2017 only (top right), gain M (bottom left) and sunglint (bottom right) soundings. N(coloc) indicates the number of GOSAT-TCCON colocations, 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 ~ 0.9). 2017 shows a smaller correlation but that is due to the limited range of XCO2 values covered in 2017 compared to the whole timeseries. This gives us confidence that our bias correction based on the retrieved albedo works correctly and takes out most of the bias.

The figure below (Fig 13) 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 3.45 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 4 co-located measurements.

Figure 13: The bias, standard deviation and # of measurements per station for gain H (top), gain M (middle) and sunglint (bottom) soundings.

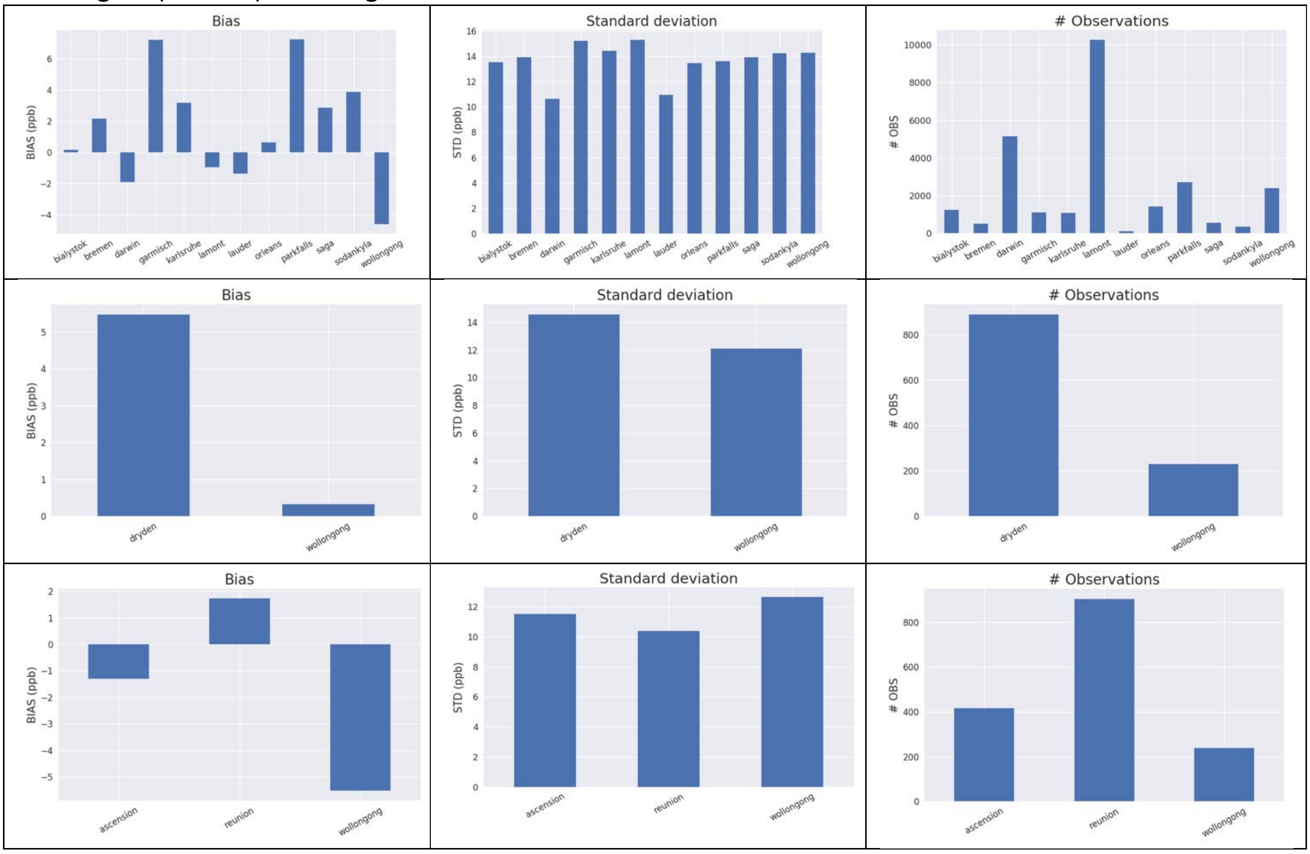
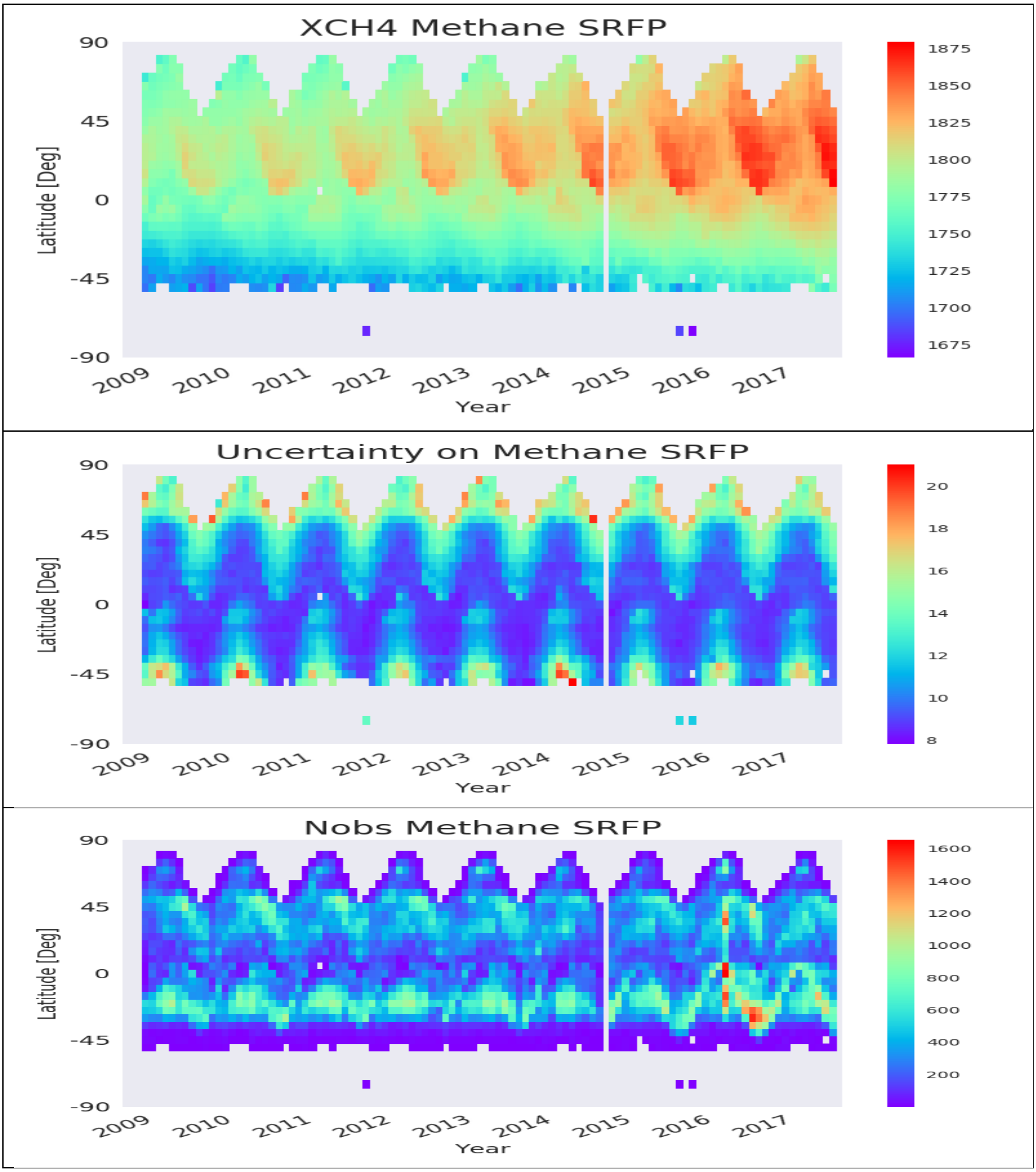


Figure 14: The CH4_GOS_SRFP global dataset in slices of 10 degrees latitude as a function of time. The increase in XCH4 concentrations during the last couple of years can clearly be seen. The gap in data coverage during Dec 2014 and Jan 2015 is due to GOSAT maintenance and testing.


XCH4 Methane SRFP
Latitude [Deg]
90
45
0
-45
-90
2009 2010 2011 2012 2013 2014 2015 2016 2017
Year
1875 1850 1825 1800 1775 1750 1725 1700 1675
Uncertainty on Methane SRFP
20 18 16 14 12 10 8
Nobs Methane SRFP
1600 1400 1200 1000 800 600 400 200

2.2.2 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. 15-19 show the timeseries 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 3.

Figure 15: Timeseries for the individual stations for gain H for CH4_GOS_SRFP

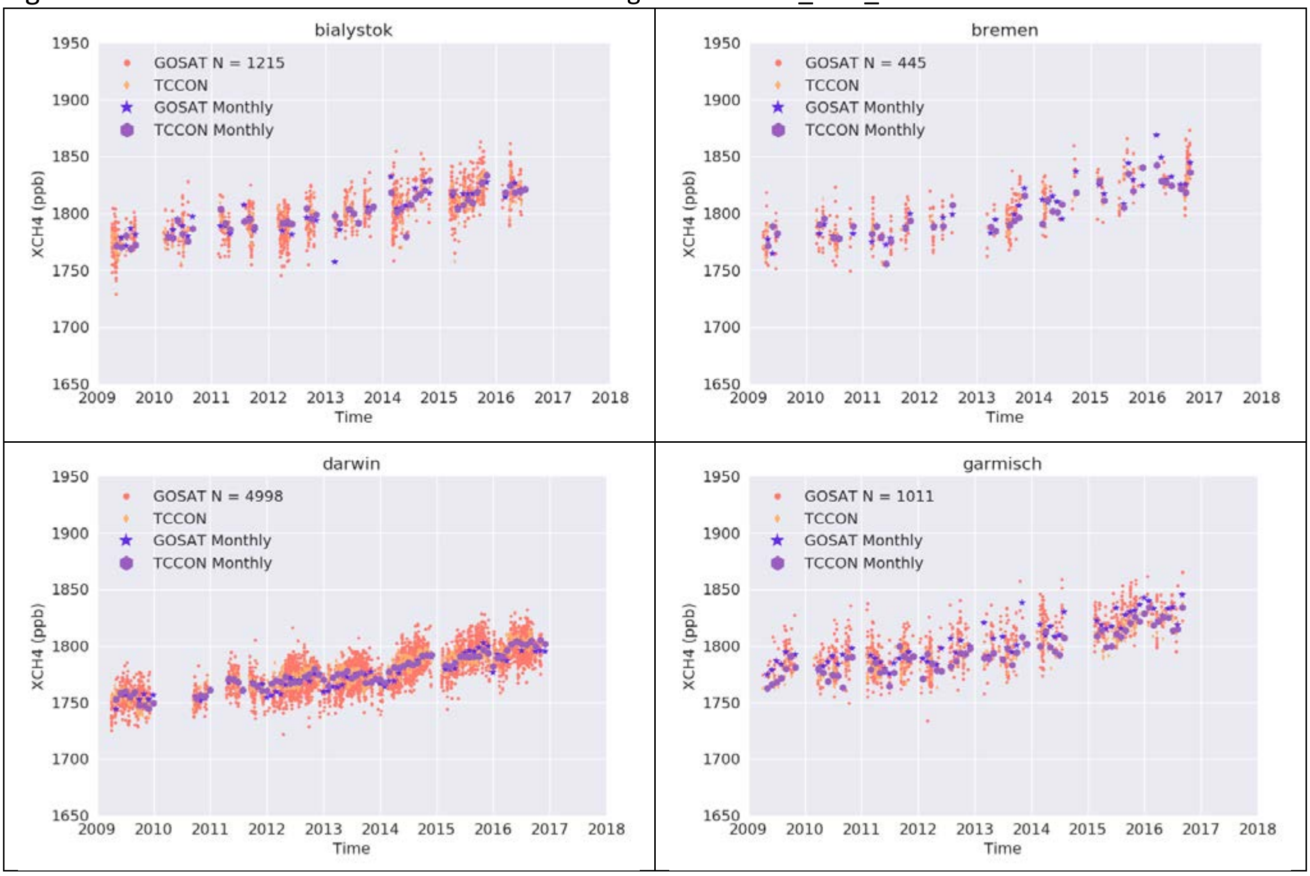


Figure 16: Timeseries for the individual stations for gain H for CH4_GOS_SRFP (continued from Fig 15).

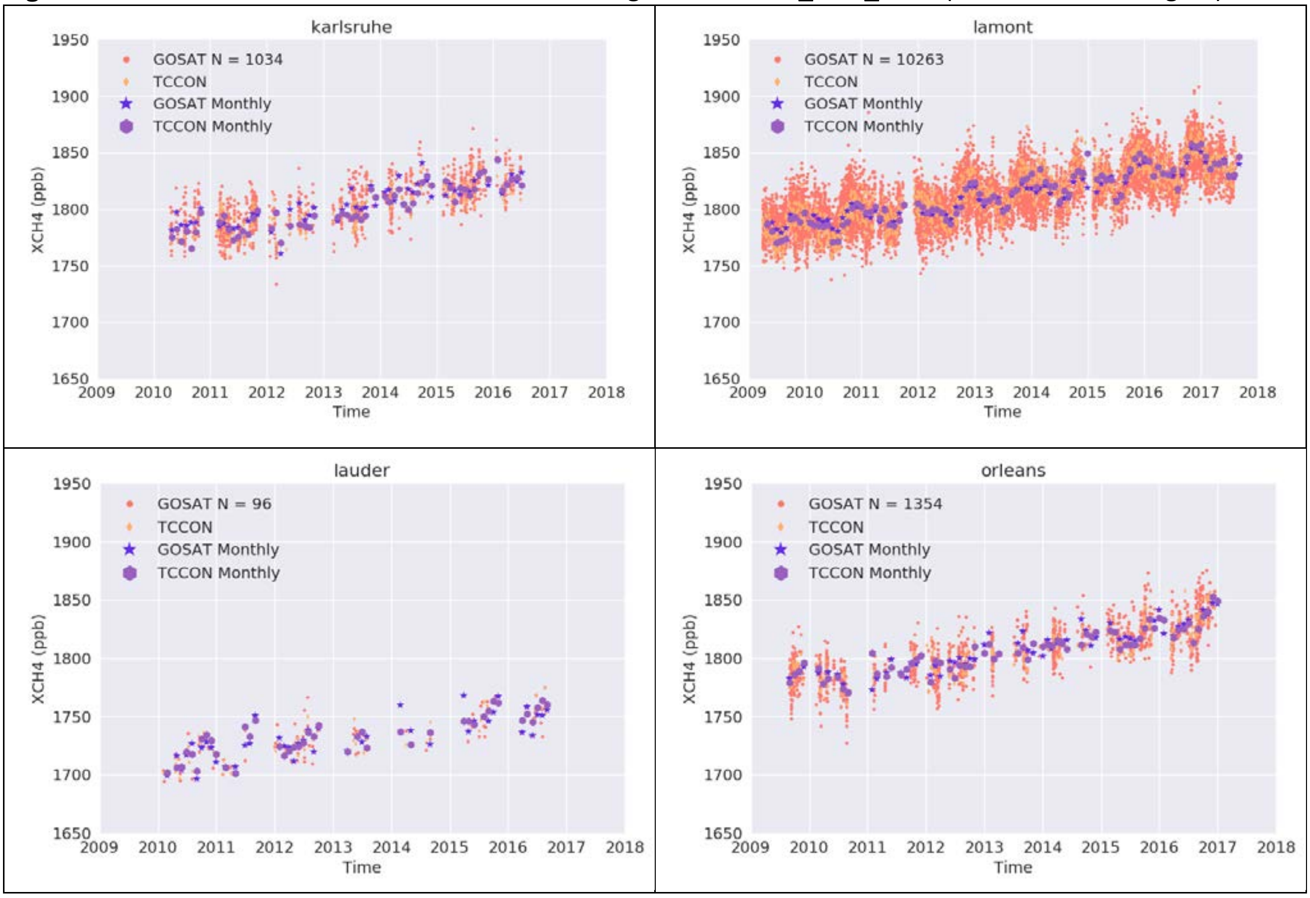
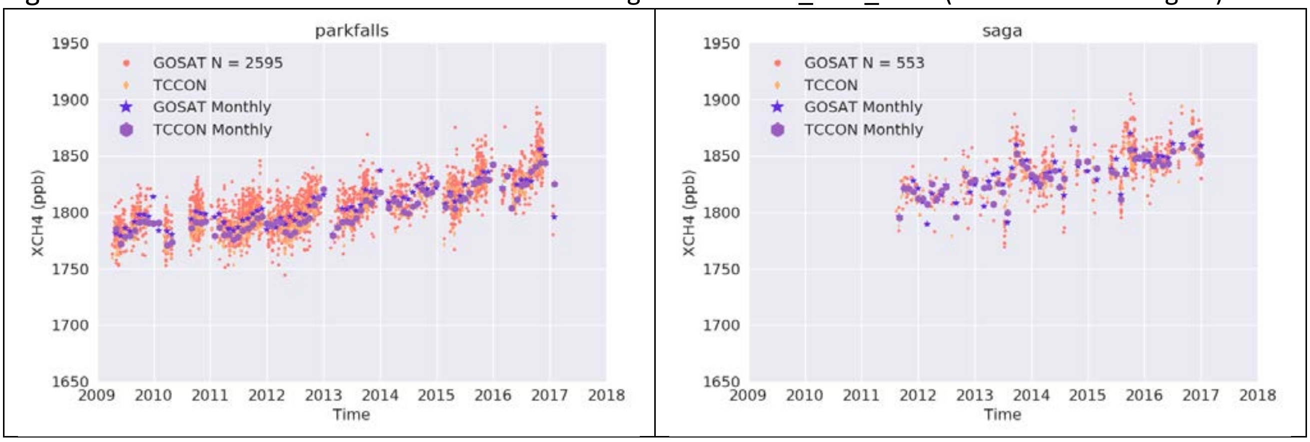


Figure 17: Timeseries for the individual stations for gain H for CH4_GOS_SRFP (continued from Fig 15).



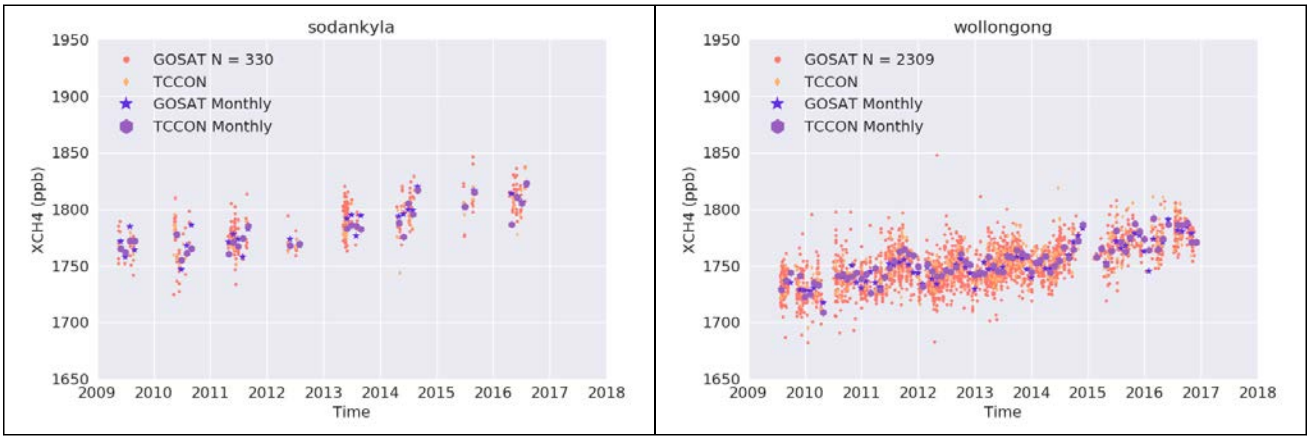


Figure 18: Timeseries for the individual stations for gain M for CH4_GOS_SRFP.

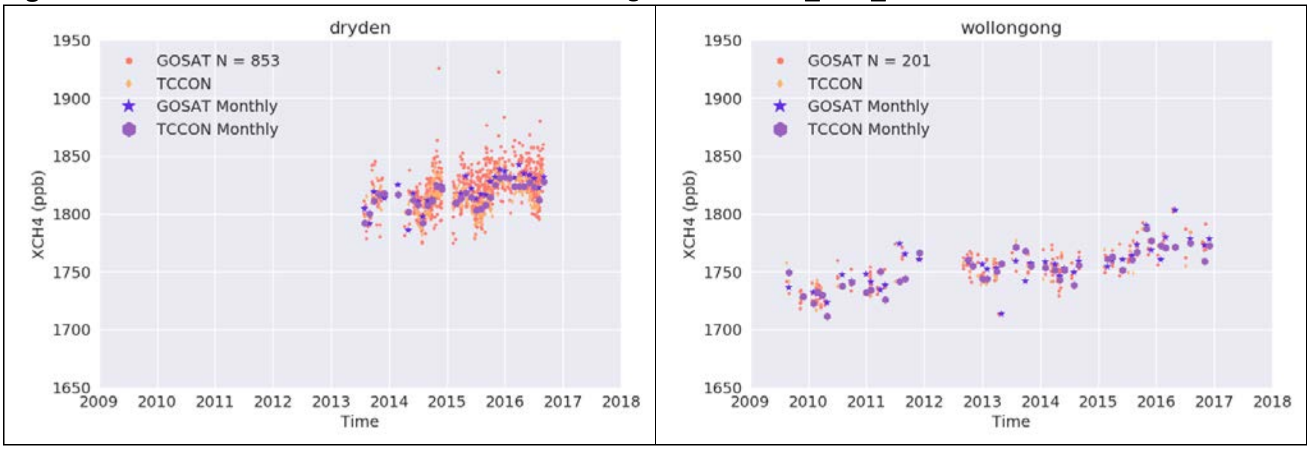
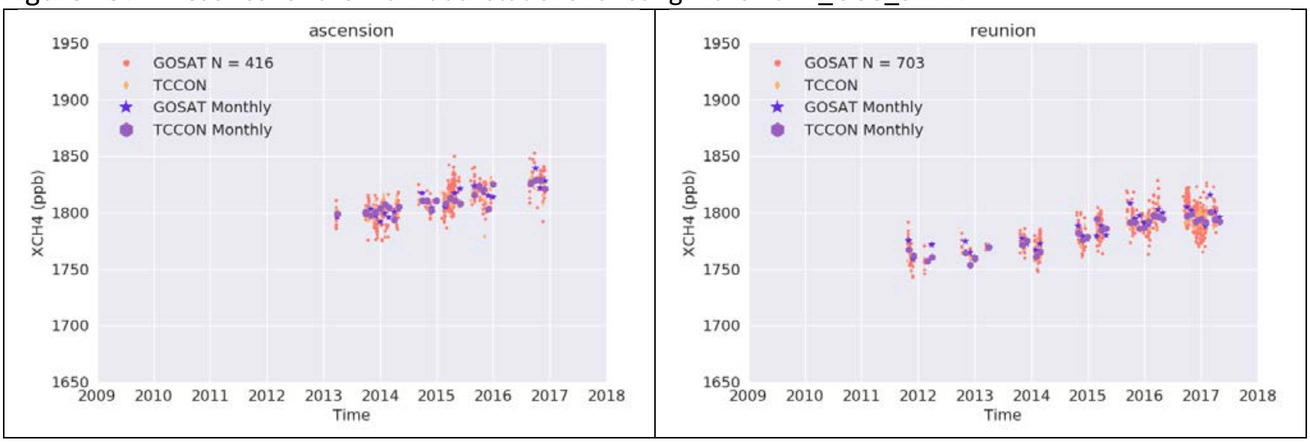
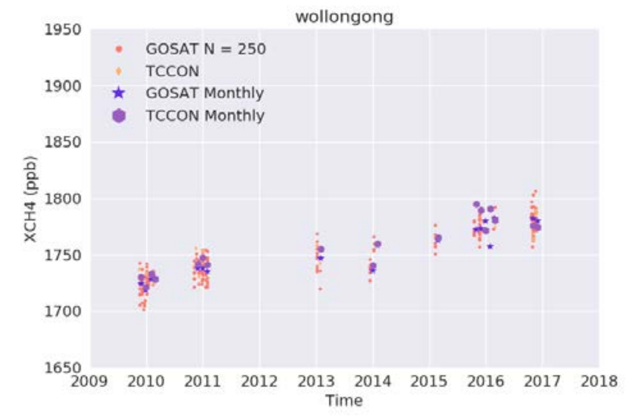


Figure 19: Timeseries for the individual stations for sunglint for CH4_GOS_SRFP.




wollongong
GOSAT N = 250
TCCON
GOSAT Monthly
TCCON Monthly
XCH4 (ppb)
1950
1900
1850
1800
1750
1700
1650
2009
2010
2011
2012
2013
2014
2015
2016
2017
2018
Time

2.2.3 Validation summary

The validation results are summarized in the table below.

Table 3 - Product Quality Summary Table for product CH4_GOS_SRFP.

Product Quality Summary Table for Product: CH4_GOS_SRFP Level: 2, Version: 2.3.8, Time period covered: 6.2009 – 12.2017				
Parameter [unit]	Achieved performance	Requirement	TR	Comments
Single measurement precision (1-sigma) in [ppb]	14.33	< 34 (T) < 17 (B) < 9 (G)	-	-
Uncertainty ratio) in [-]: Ratio reported uncertainty to standard deviation of satellite-TCCON difference	1.22	-	-	No requirement but value close to unity expected for a high quality data product.
Mean bias [ppb]	-0.34	-	-	No requirement but value close to zero expected for a high quality data product.
Accuracy: Relative systematic error [ppb]	Spatial – spatiotemporal: 3.45 – 4.54	< 10	Probability that accuracy TR is met: 100 %	-
Stability: Linear bias trend [ppb/year]	-0.57 +/- 0.19 (1-sigma)	< 3	Probability that stability TR is met: 100 %	-
Stability: Year-to-year bias variability [ppb/year]	5.67 +/- 1.83 (1-sigma)	< 3	-	-

3. Application(s) specific assessments

No application specific assessments have been carried out.

4. Compliance with user requirements

For the CO2_GOS_SRFP product we reached a 65 % chance that the TR is met for Accuracy and a 100 % chance the TR is met for Stability.
For the CH4_GOS_SRFP product both Accuracy and Stability achieved a TR of 100 %.

References

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