FRM4GHG

Fiducial Reference Measurements for Greenhouse Gases

Validation Report

Deliverable: D6 of Phase 2

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Proposal from February 16, 2016 plus comments from May 27, 2016

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1 Document change record

Issue	Date	Item	Comment
V0.0	2018-09-26	–	First validation results also shown at the ESA-ESRIN meeting
V0.1	2019-02-25	–	Update of the validation results using one year of data from 2018 measurements
V0.2	2020-04-24	–	Update of the validation results using two years of data from 2018-2019 measurements
V1.0	2020-07-02	–	Final reporting of the validation results

2 Access list

This document is a deliverable "D6: Validation Report" created for phase 2 of the project FRM4GHG to be submitted to ESA. The document will be a publicly accessible document and can be downloaded from the project webpage http://frm4ghg.aeronomie.be.

3 Document structure

Section 4 presents the purpose of the document.

Section 5 'Validation results' presents the validation results of methane (CH_4) and carbon monoxide (CO) data products from Sentinel-5 Precursor satellite using data from the FRM4GHG campaign.

Section 6 & 7 'Applicable and reference documents' presents a list of all applicable and reference documents.

Section 8 'Reference for software/tool mentioned' presents a list of all software/tool mentioned in this document.

4 Purpose

This document focuses on the S-5P methane and carbon monoxide validation using FRM4GHG data. The co-location criteria used for the validation study are discussed in details. The validation results showing the systematic and random uncertainty observed for the dataset from each instrument are shown and compared to the validation results using TCCON data.

5 Validation results

Sentinel-5 Precursor (S-5P) was launched successfully on 13 October 2017. It has a push broom configuration and a wide swath of 108° that corresponds to 2600 km on the earth surface. It provides a daily global coverage of methane (CH_4) and carbon monoxide (CO), amongst other species, with a horizontal resolution of 7 x 7 km^2. Since 6th of August 2019, the resolution has been further improved to 5.5 x 7 km^2. The Sun-synchronous polar orbit of S-5P provides an equator crossing time of 13:30 local solar time.

In this document, the validation results of the S-5P methane and carbon monoxide products using remote sensing data from the FRM4GHG campaign performed at the Sodankylä, Wollongong and

Darwin TCCON sites are presented. The requirements for the S-5P CH_4 product: Systematic uncertainty (bias) of less than 1.5% and random uncertainty (std) of less than 1%. The requirements for the S-5P CO product: Bias of less than 15% and std of <10%. Following the recommendations of the Product Readme File (PRF), S-5P data with a qa_value above 0.5 are used for the validation study.

The S-5P offline (OFFL) and reprocessed (RPRO) overpass files for the Sodankylä, Wollongong and Darwin sites are provided by the Payload Data Ground Segment (PDGS) at Deutsches Zentrum für Luft- und Raumfahrt (DLR) and are downloaded from the Copernicus data hub and Mission Performance Centre (MPC). The version number of the S-5P files and the corresponding orbit numbers for methane and carbon monoxide are indicated in Table 1. The S-5P level 2 (L2) data contains two XCH_4 column values: the standard retrieved product and a bias corrected product. The validation results with the bias corrected product are discussed in this report.

Table 1: S-5P methane and carbon monoxide product stream and processor version (RPRO reprocessed and OFFL offline) used for this report.

Product	Stream	Version	In operation from orbit no., date	In operation till orbit no., date
L2_CH4	RPRO	01.02.02 01.03.01 01.03.02	0657, 2017-11-28 2818, 2018-04-30 2463, 2018-04-04	5346, 2018-10-25 5832, 2018-11-28 2477, 2018-04-05
	OFFL	01.02.02 01.03.00 01.03.01 01.03.02	5833, 2018-11-28 7425, 2019-03-20 7907, 2019-04-23 8812, 2019-06-26	7424, 2019-03-20 7906, 2019-04-23 8814, 2019-06-26 current version
L2_CO	RPRO	01.02.02 01.03.01 01.03.02	5236, 2018-10-17 2818, 2018-04-30 2463, 2018-04-04	5346, 2018-10-25 5832, 2018-11-28 2477, 2018-04-05
	OFFL	01.02.00 01.02.02 01.03.00 01.03.01 01.03.02	5346, 2018-10-25 5833, 2018-11-28 7425, 2019-03-20 7907, 2019-04-23 8815, 2019-06-26	5832, 2018-11-28 7424, 2019-03-20 7906, 2019-04-23 8814, 2019-06-26 current version

Further details regarding the S-5P and the data products are available in details in the Product Readme File (PRF), Product User Manual (PUM) and Algorithm Theoretical Basis Document (ATBD) associated with the respective data products, all available on https://sentinels.copernicus.eu/web/sentinel/technical-guides/sentinel-5p/products-algorithms and in the files indicated in the applicable documents.

5.1 Validation results for S-5P methane product

The S-5P methane observations co-located with the ground-based remote sensing measurements are found by selecting all filtered S-5P pixels within a radius of 100 km around the TCCON stations at Sodankylä, Wollongong and Darwin and with a maximal time difference of one hour. The selection criterion is identical to the one used for the operational validation of the S-5P methane products using

global TCCON data. The 1h time interval can also be justified for the low-resolution instruments by noting that the ground-based remote sensing instruments of TCCON and other low-resolution instruments tested during the FRM4GHG campaign acquire a sufficient amount of measurements to be statistically relevant. All instruments tested during the FRM4GHG campaign, i.e., EM27/SUN, VERTEX70, IRCUBE and Laser Heterodyne spectro-Radiometer (LHR), provided methane. However, the LHR inter-comparison results show that the data have a large scatter and biases with a strong diurnal variation relative to the TCCON and other Fourier transform spectrometer (FTS) instruments. Therefore, the data from the LHR has not been used for the S-5P validation. The low-resolution data used the same a priori profiles as the TCCON for the processing thereby removing any difference between the datasets due to a priori mismatch.

The current validation results are based on the S-5P and reference measurements available at the time of this analysis, which yield comparison pairs from March 2018 until December 2019. The increased spatial resolution from 7 km to 5.5 km along track since 6 August 2019 (orbit 9388) did not change the performance of the S-5P methane product as mentioned in the S5P Mission Performance Centre Quarterly Validation Report (ROCVR #06). Therefore, the full time period of the measurements performed between 2018 and 2019 FRM4GHG campaign is used for the validation and are presented here.

5.1.1 S-5P XCH_4 validation using EM27/SUN data

The EM27/SUN performed measurements at the Sodankylä TCCON site during 2017 – 2019 in the period between spring (March) and autumn (October) of each year. Due to the location of the site at a high latitude, it is not possible to perform solar absorption measurements during the late autumn until early spring as the sun is either too low or even below the horizon.

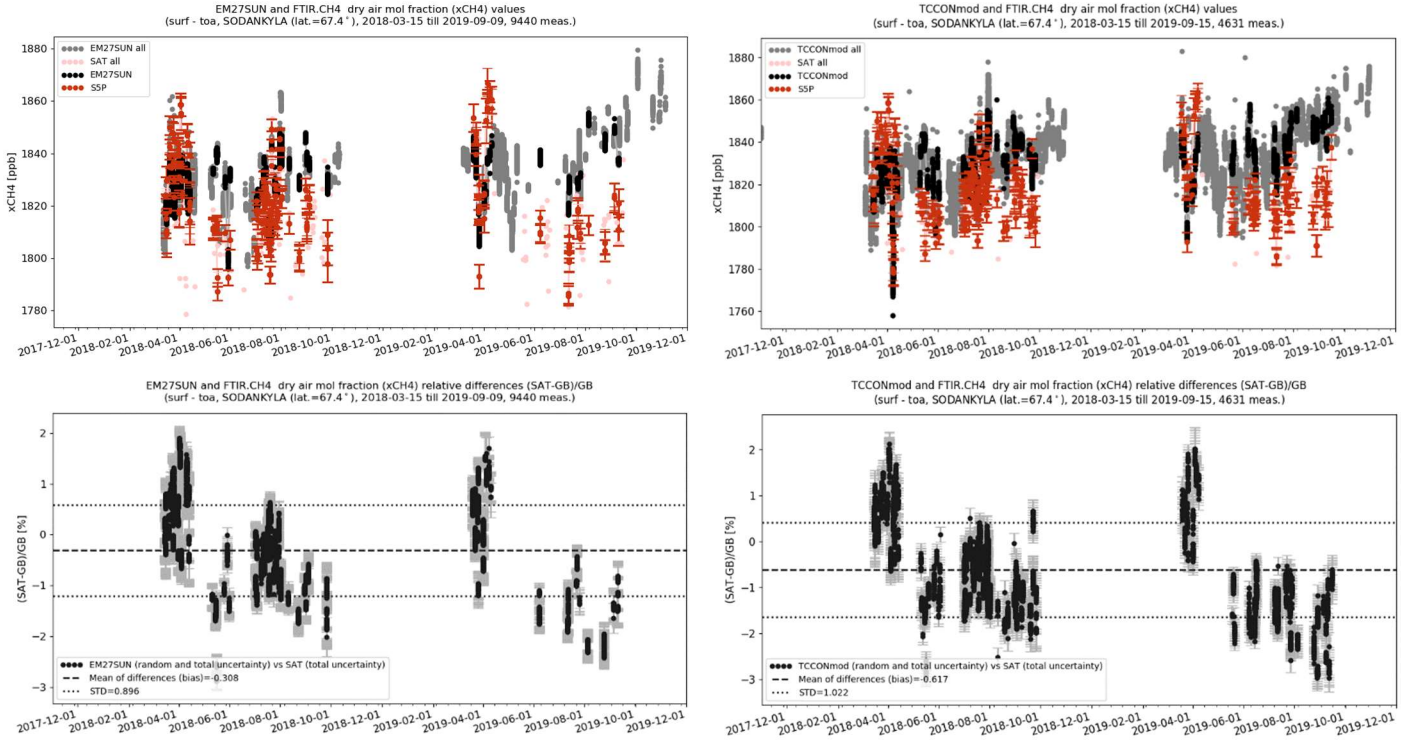

Figure 1: Top-left: Time series of XCH_4 plotted for EM27/SUN (grey) and S-5P (light red) for the year 2018 and 2019. The co-located XCH_4 from EM27/SUN (black) and S-5P (red) are overlaid on the same plot. Top-right: The same plot as the top-left but with TCCON dataset as the reference. Bottom-left: Time series of the XCH_4 relative difference ((SAT – GB)/GB) between the S-5P and EM27/SUN data as reference showing the bias of the S-5P XCH_4 product in relation to the EM27/SUN data. Bottom-right: The same plot as the bottom-left but with TCCON dataset as the reference.

The S-5P and EM27/SUN XCH_4 data from the Sodankylä campaign during 2018 and 2019 are plotted in Figure 1. The top figures show the time series with dark red and black points showing the co-located points and error bars showing the scatter in the data. The grey and light-red points show the time series of all measurements. The bottom figures show the XCH_4 relative difference ((SAT – GB)/GB) between the satellite and the reference ground-based instrument. The left panel plots are for S-5P validation results with EM27/SUN data used as the reference ground-based dataset and the right panel plots are with TCCON data used as the reference ground-based dataset. The validation results with the EM27/SUN data show similar pattern as the validation results with the TCCON data. The springtime results show a positive bias, which makes a jump later in the year, around May, then showing a negative bias. This jump in the bias is seen for both the years. During the March – May period, the airmass above the site is quite often from polar vortex conditions. This is not so well represented by the a priori and therefore there can be large differences between the a priori used for the retrieval and the true atmospheric state. As the averaging kernel of the instruments differ, the difference of the a priori from the true state will influence the retrieval results differently. The second reason for the difference is related to the change in the surface albedo due to the change of the ice/snow-covered surface to snow free condition during the year. The standard S-5P XCH_4 product shows a bias dependence on the surface albedo. The bias-correction as currently performed (ref.: Figure 5 of ATBD; https://sentinels.copernicus.eu/documents/247904/2476257/Sentinel-5P-TROPOMI-ATBD-Methane-retrieval) is not ideal for the low-surface albedo conditions. Therefore, this can contribute to the residual bias seen in the S-5P bias-corrected product and the corresponding change during the transition from snow cover to snow free surface leading to a change in the surface albedo.

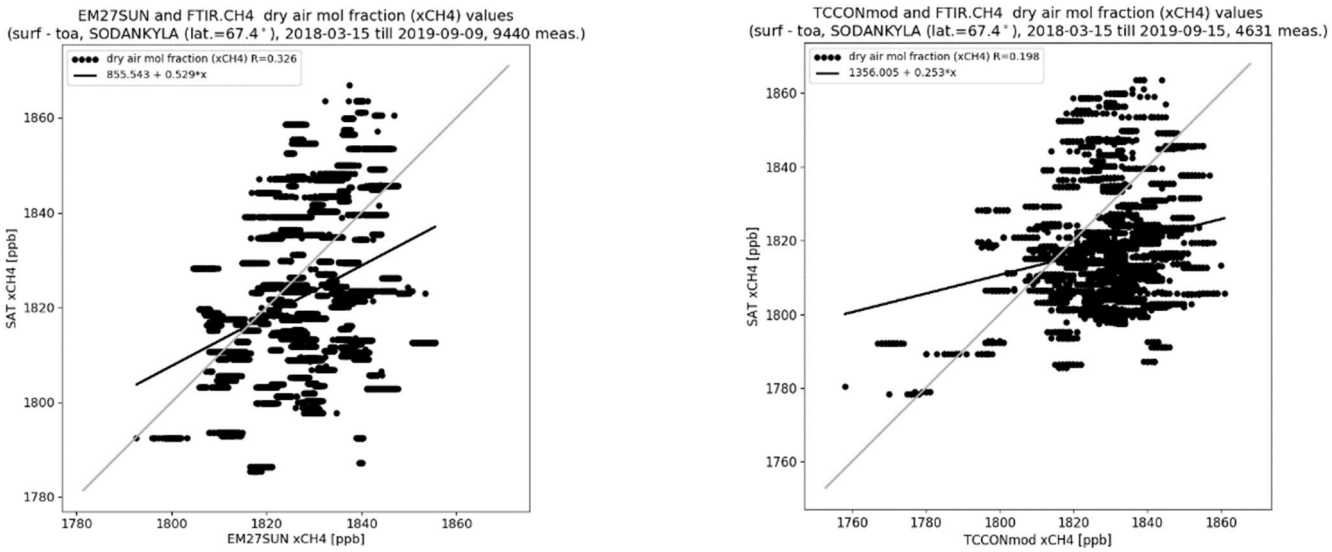

Figure 2: Left: Correlation plot for XCH_4 data between co-located S-5P data and EM27/SUN data for the 2018 – 2019 period. Right: Correlation plot for XCH_4 data between co-located S-5P data and TCCON data for the same period.

Table 2: Statistics of S-5P XCH_4 validation using EM27/SUN data and TCCON data as reference.

Validation type	Bias %	STD %	R
EM27/SUN vs TCCON	0.05 (1 ppb)	0.22 (4 ppb)	0.943
S-5P vs EM27/SUN	-0.31	0.9	0.326
S-5P vs TCCON	-0.62	1.02	0.198

The correlation plots for XCH_4 between the S-5P vs EM27/SUN data and those between the S-5P vs TCCON data are shown in Figure 2. The two plots show similar behaviour, the differences are due to the data representative differences between the EM27/SUN and TCCON datasets. The TCCON instrument operation was automatic and therefore recorded measurements on every occasion. The EM27/SUN was setup outside the FRM4GHG container on a daily basis on rain free days. The EM27/SUN vs TCCON comparison results show a very small bias with a low scatter of 0.05% ± 0.22% with a high correlation of 0.943. The S-5P vs EM27/SUN validation results show a bias of -0.31% ± 0.9% with a correlation of 0.326. The S-5P vs TCCON validation results show a bias of -0.62% ± 1.02% with a correlation of 0.198. The bias values between the two datasets are very close to each other whereby the small difference is due to the data representative differences between the EM27/SUN and TCCON. The statistics of the results are shown in Table 1. The results confirm that the bias and the std for S-5P XCH_4 product are compliant with the mission requirement.

5.1.2 S-5P XCH_4 validation using VERTEX70 data

The VERTEX70 performed measurements at the Sodankylä TCCON site during 2017 – 2019.

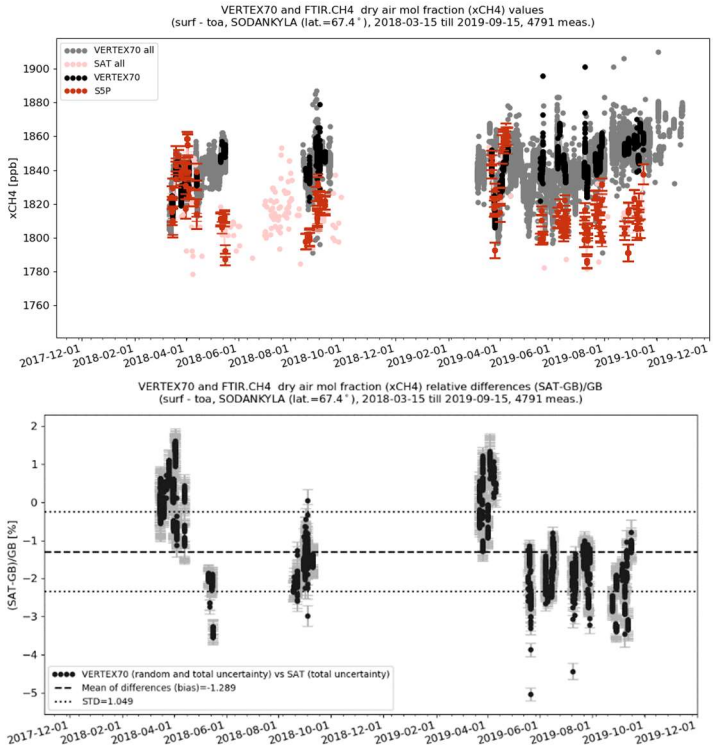

Figure 3: Top: Time series of XCH_4 plotted for VERTEX70 (grey) and S-5P (light red) for the year 2018 and 2019. The co-located XCH_4 from VERTEX70 (black) and S-5P (red) are overlaid on the same plot. Bottom: Time series of the XCH_4 relative difference ((SAT – GB)/GB) between the S-5P and VERTEX70 data as reference showing the bias of the S-5P XCH_4 product in relation to the VERTEX70 data.

The S-5P and VERTEX70 XCH_4 data from the Sodankylä campaign during 2018 and 2019 are plotted in Figure 3. The top figure shows the time series with dark red and black points showing the co-located points and error bars showing the scatter in the data. The grey and light-red points show the time series of all measurements. The bottom figure shows the XCH_4 relative difference ((SAT – GB)/GB) between the satellite and the reference ground-based instrument. The validation results with the VERTEX70 data show similar pattern as the validation results with the TCCON data. The springtime results show a positive bias which makes a jump later in the year, around May, then showing a negative bias. This jump in the bias is seen for both the years 2018 and 2019.

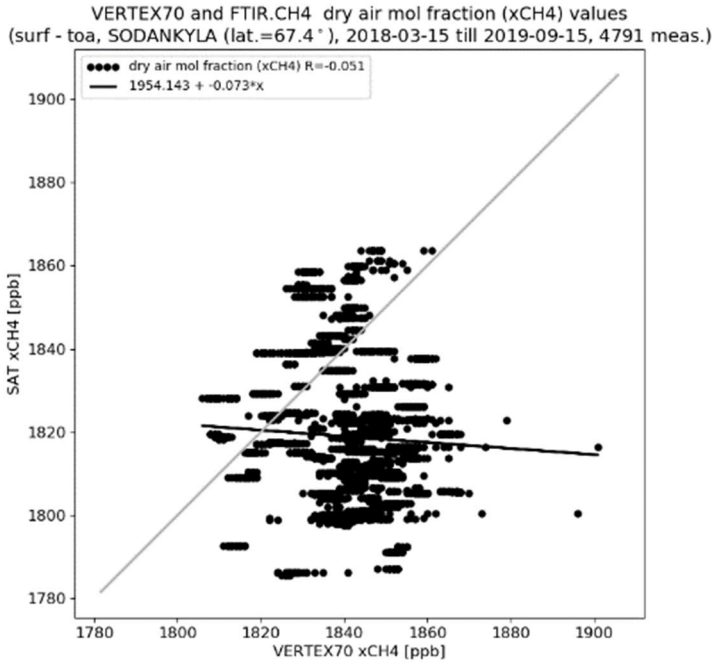

Figure 4: Correlation plot for XCH_4 data between co-located S-5P data and VERTEX70 data for the 2018 – 2019 period.

Table 3: Statistics of S-5P XCH_4 validation using VERTEX70 data and TCCON data as reference.

Validation type	Bias %	STD %	R
VERTEX70 vs TCCON	0.5 (9 ppb)	0.16 (3 ppb)	0.971
S-5P vs VERTEX70	-1.29	1.05	-0.051
S-5P vs TCCON	-0.62	1.02	0.198

The correlation plot for XCH_4 between the S-5P vs VERTEX70 is shown in Figure 4. The plot shows similar behaviour as the S-5P vs TCCON correlation plot and the differences are due to the data representative differences between the VERTEX70 and TCCON datasets. The VERTEX70 instrument has some instrumental modifications to test different detectors in 2018. These measurements are not included, as the results did not show any improvement in comparison to the optimized setting as selected in 2017. The VERTEX70 vs TCCON comparison results show a bias of 0.5% with a low scatter of 0.22% and a high correlation of 0.971. No instrument specific scaling factor is applied to the

VERTEX70 data. The S-5P vs VERTEX70 validation results show a bias of -1.29% ± 1.05% with a correlation of -0.051. The S-5P vs TCCON validation results show a bias of -0.62% ± 1.02% with a correlation of 0.198. The statistics of the results are shown in Table 3. The bias between the VERTEX70 vs TCCON is also reflected in the bias seen between the S-5P vs VERTEX70. Once a scaling factor for the VERTEX70 is applied, the results are similar to the bias seen between the S-5P vs TCCON. The results confirm that the bias and the std for S-5P XCH_4 product are compliant with the mission requirement.

5.1.3 S-5P XCH_4 validation using IRCUBE data

The IRCUBE performed measurements at the Sodankylä TCCON site during 2017 – 2018. It was then shipped to Australia for further campaign measurements. It performed measurements at the Wollongong TCCON site during 17 January to 23 August 2019 and at the Darwin TCCON site during 12 September to 31 December 2019. The S-5P XCH_4 validation results using the IRCUBE data from the three sites are shown in this report.

S5P – XCH_4 validation using IRCUBE data from the Sodankylä campaign during 2018.

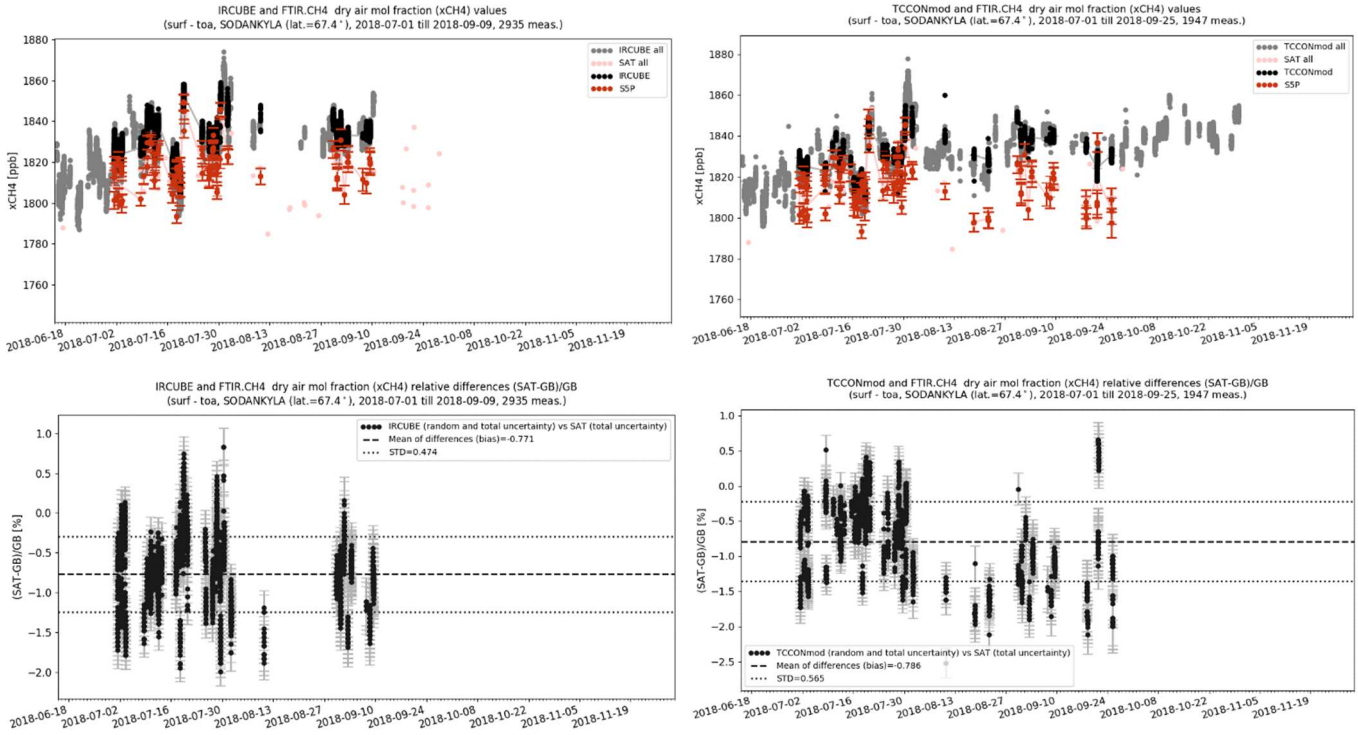

Figure 5: Top-left: Time series of XCH_4 plotted for IRCUBE (grey) and S-5P (light red) for the year 2018. The co-located XCH_4 from IRCUBE (black) and S-5P (red) are overlaid on the same plot. Top-right: The same plot as the top-left but with TCCON dataset as the reference. Bottom-left: Time series of the XCH_4 relative difference ((SAT – GB)/GB) between the S-5P and IRCUBE data as reference showing the bias of the S-5P XCH_4 product in relation to the IRCUBE data. Bottom-right: The same plot as the bottom-left but with TCCON dataset as the reference.

The S-5P and IRCUBE XCH_4 data from the Sodankylä campaign during 2018 are plotted in Figure 5. The top figure shows the time series with dark red and black points showing the co-located points and error bars showing the scatter in the data. The grey and light-red points show the time series of all measurements. The bottom figure shows the XCH_4 relative difference ((SAT – GB)/GB) between the satellite and the reference ground-based instrument. The validation results with the IRCUBE data show similar patterns as the validation results with the TCCON data.

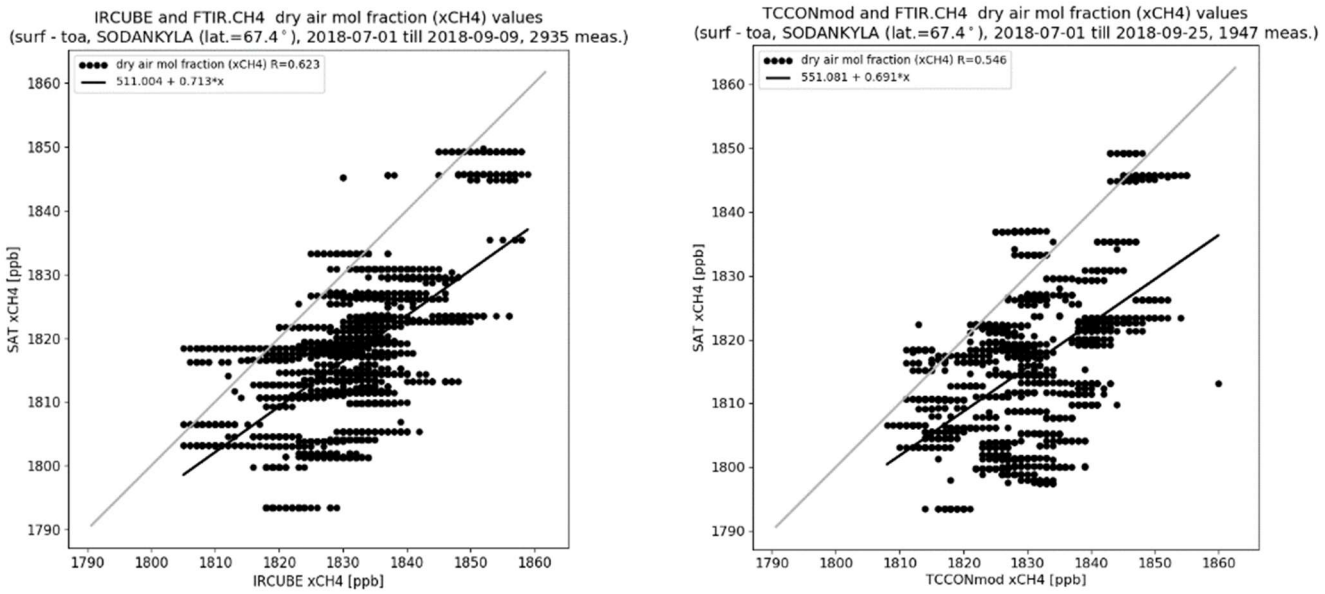

Figure 6: Left: Correlation plot for XCH_4 data between co-located S-5P data and IRCUBE data for the year 2018. Right: Correlation plot for XCH_4 data between co-located S-5P data and TCCON data for the same period.

Table 4: Statistics of S-5P XCH_4 validation using IRCUBE data and TCCON data as reference from Sodankylä site.

Validation type	Bias %	STD %	R
IRCUBE vs TCCON	-0.054 (-1 ppb)	0.272 (5 ppb)	0.911
S-5P vs IRCUBE	-0.771	0.474	0.623
S-5P vs TCCON	-0.786	0.565	0.546

The correlation plots for XCH_4 between the S-5P vs IRCUBE data and those between the S-5P vs TCCON data are shown in Figure 6. The two plots show similar behaviour, the differences are due to the data representative differences between the IRCUBE and TCCON datasets. The IRCUBE vs TCCON comparison results show a very small bias with a low scatter of -0.054% ± 0.272% with a high correlation of 0.911. The S-5P vs IRCUBE validation results show a bias of -0.771% ± 0.474% with a correlation of 0.623. The S-5P vs TCCON validation results show a bias of -0.786% ± 0.565% with a correlation of 0.546. The bias values between the two datasets are very close to each other whereby the small difference is due to the data representative differences between the IRCUBE and TCCON. The statistics of the results are also shown in Table 4. The results confirm that the bias and the std for S-5P XCH_4 product are compliant with the mission requirement.

S5P – XCH_4 validation using IRCUBE data from the Wollongong campaign during 2019.

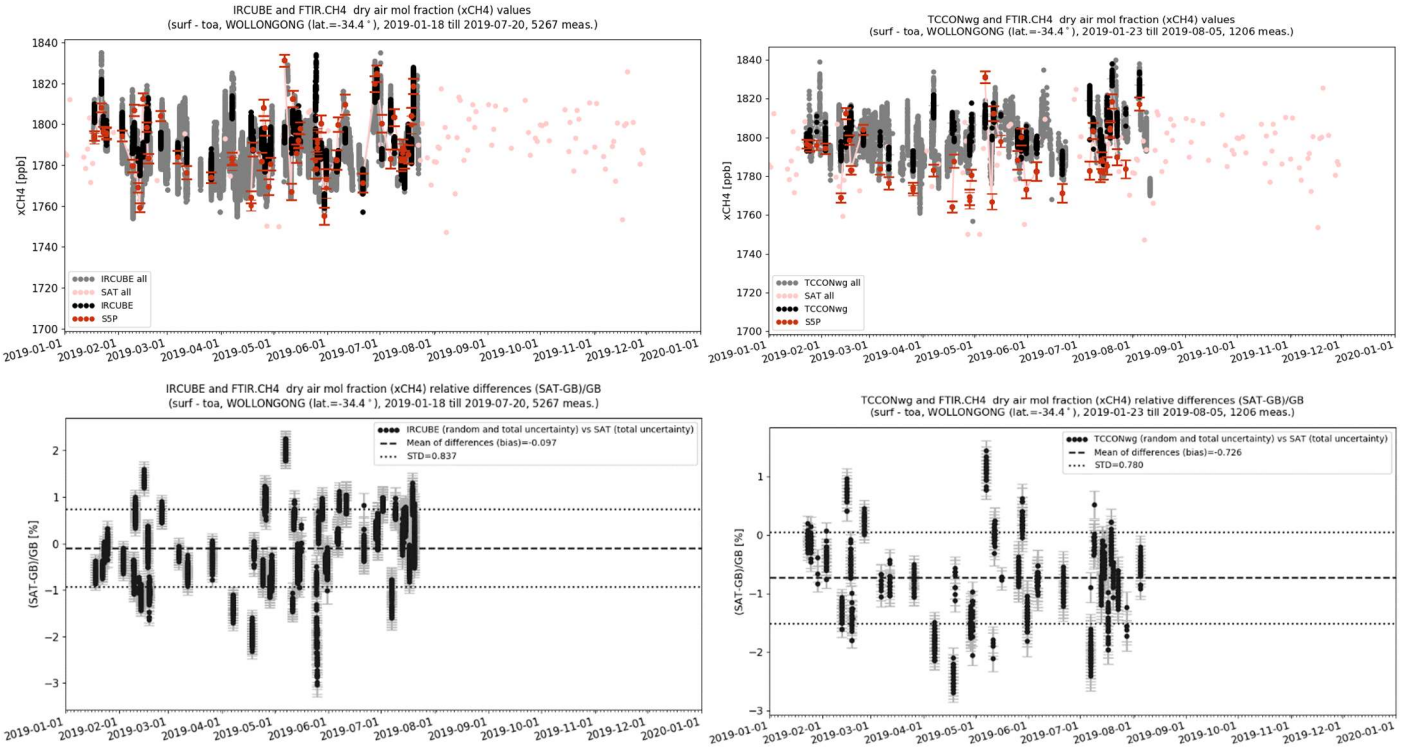

Figure 7: Top-left: Time series of XCH_4 plotted for IRCUBE (grey) and S-5P (light red) at the Wollongong site for the year 2019. The co-located XCH_4 from IRCUBE (black) and S-5P (red) are overlaid on the same plot. Top-right: The same plot as the top-left but with TCCON dataset as the reference. Bottom-left: Time series of the XCH_4 relative difference ((SAT – GB)/GB) between the S-5P and IRCUBE data as reference showing the bias of the S-5P XCH_4 product in relation to the IRCUBE data. Bottom-right: The same plot as the bottom-left but with TCCON dataset as the reference.

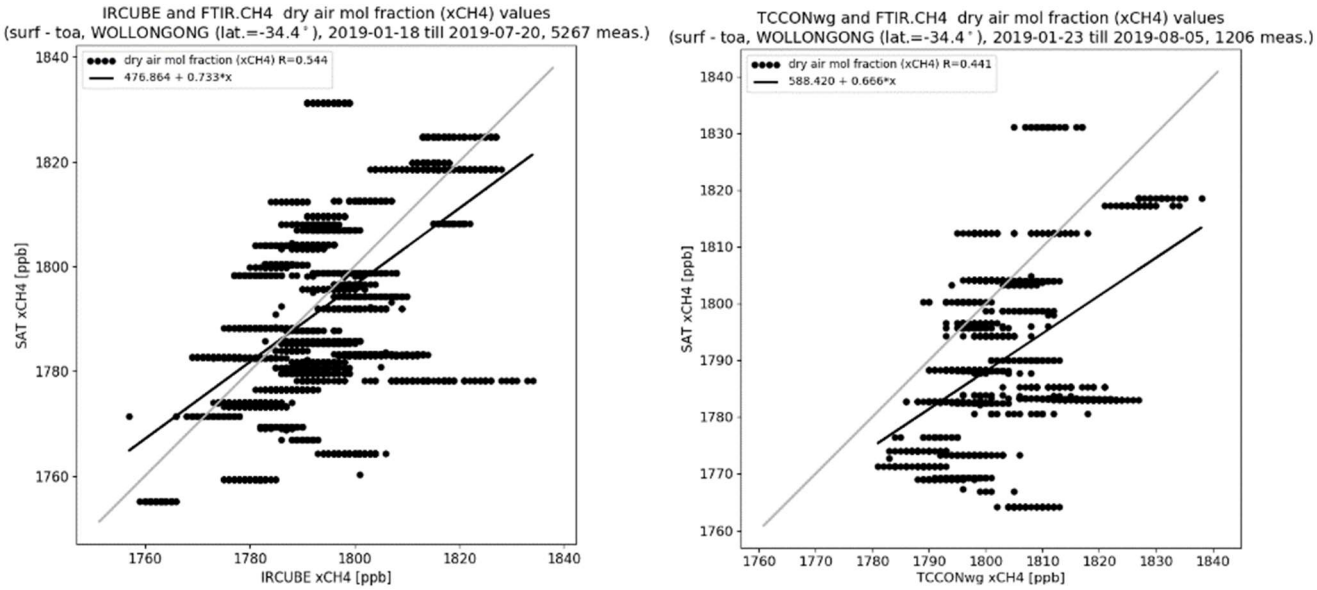

Figure 8: Left: Correlation plot for XCH_4 data between co-located S-5P data and IRCUBE data at the Wollongong site for the year 2019. Right: Correlation plot for XCH_4 data between co-located S-5P data and TCCON data for the same period.

Table 5: Statistics of S-5P XCH_4 validation using IRCUBE data and TCCON data as reference from Wollongong site.

Validation type	Bias %	STD %	R
IRCUBE vs TCCONwg	-0.707 (-13 ppb)	0.272 (5 ppb)	0.867
S-5P vs IRCUBE	-0.097	0.837	0.544
S-5P vs TCCONwg	-0.726	0.780	0.441

The S-5P XCH_4 validation results using IRCUBE data at the Wollongong site for the year 2019 are plotted in the left panel plots of Figure 7. The validation results using TCCON data for the same time period is shown in the right panel plots of Figure 7. The corresponding correlation plots are show in Figure 8. The validation plots with the IRCUBE show similar pattern as the validation results with the TCCON data. The IRCUBE vs TCCON comparison results show a bias of -0.707% with a low scatter of 0.272% and with a high correlation of 0.867. The bias seen in the IRCUBE is higher for the Wollongong measurements as compared to the Sodankylä. The S-5P vs IRCUBE validation results show a bias of -0.097% ± 0.837% with a correlation of 0.544. The S-5P vs TCCON validation results show a bias of -0.726% ± 0.780% with a correlation of 0.441. The bias between the IRCUBE vs TCCON is also reflected in the bias seen between the S-5P vs IRCUBE. The statistics of the results are also shown in Table 5. The results confirm that the bias and the std for S-5P XCH_4 product are compliant with the mission requirement.

S5P – XCH_4 validation using IRCUBE data from the Darwin campaign during 2019.

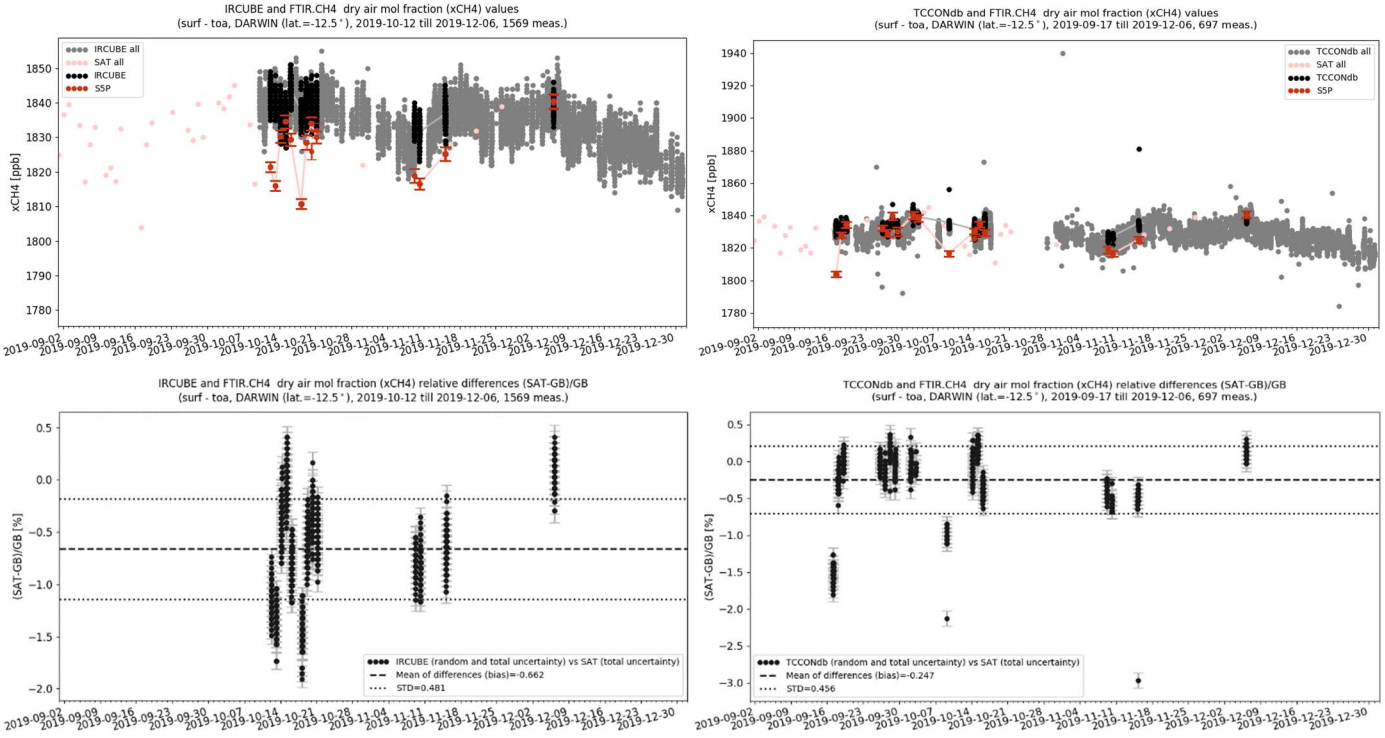

Figure 9: Same plots as Figure 7 but for measurements performed with the IRCUBE and the TCCON at the Darwin site.

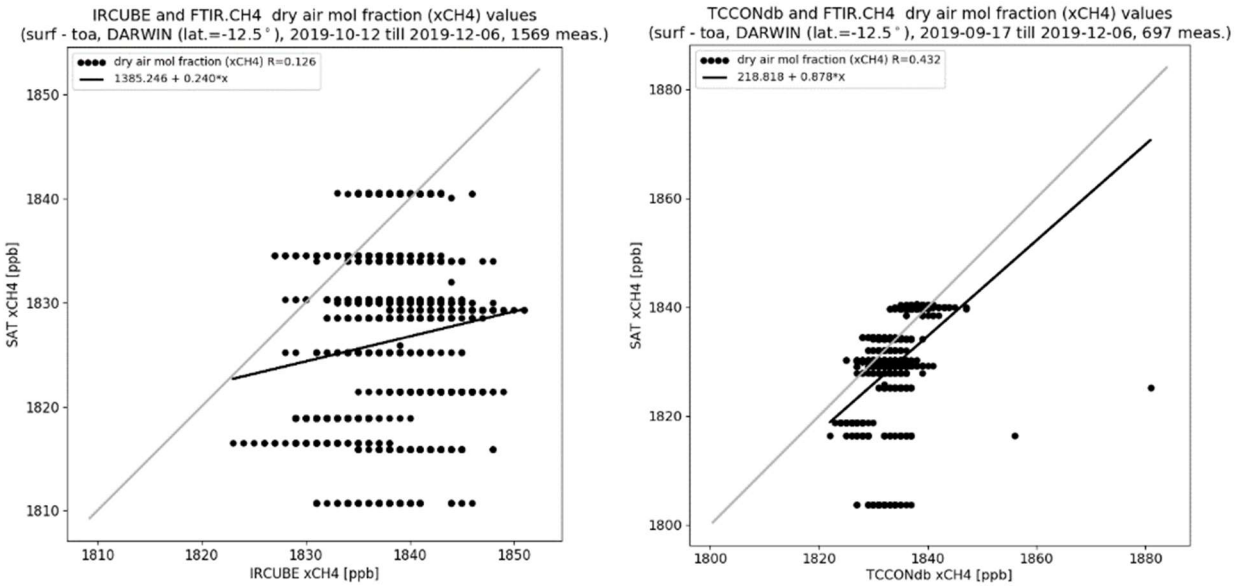

Figure 10: Left: Correlation plot for XCH_4 data between co-located S-5P data and IRCUBE data at the Darwin site for the year 2019. Right: Correlation plot for XCH_4 data between co-located S-5P data and TCCON data for the same period.

Table 6: Statistics of S-5P XCH_4 validation using IRCUBE data and TCCON data as reference from Darwin site.

Validation type	Bias %	STD %	R
IRCUBE vs TCCONdb	0.109 (2 ppb)	0.163 (3 ppb)	0.808
S-5P vs IRCUBE	-0.662	0.481	0.126
S-5P vs TCCONbd	-0.247	0.456	0.432

The S-5P XCH_4 validation results using IRCUBE data at the Darwin site for the year 2019 are plotted in the left panel plots of Figure 9. The validation results using TCCON data for the same time period is shown in the right panel plots of Figure 9. The corresponding correlation plots are show in Figure 10. The validation plots with the IRCUBE show similar patterns as the validation results with the TCCON data. The IRCUBE vs TCCON comparison results show a bias of 0.109% with a low scatter of 0.163% and with a correlation of 0.808. The bias seen in the IRCUBE for the Darwin site is not as high as for the Wollongong site and is comparable to the Sodankylä site. The S-5P vs IRCUBE validation results show a bias of -0.662% ± 0.481% with a high correlation of 0.126. The S-5P vs TCCON validation results show a bias of -0.247% ± 0.456% with a correlation of 0.432. The bias between the IRCUBE vs TCCON is also reflected in the bias seen between the S-5P vs IRCUBE. The statistics of the results are also shown in Table 6. The results confirm that the bias and the std for S-5P XCH_4 product are compliant with the mission requirement.

5.2 Validation results for S-5P carbon monoxide product

The S-5P carbon monoxide observations co-located with the ground-based remote sensing measurements are found by selecting all filtered S-5P pixels within a radius of 50 km around the TCCON stations at Sodankylä and with a maximal time difference of one hour. The selection criterion is identical to the one used for the operational validation of the S-5P carbon monoxide product using global TCCON data. The 1h time interval can also be justified for the low-resolution instruments by noting that the ground-based remote sensing instruments of TCCON and other low-resolution instruments tested during the FRM4GHG campaign acquire a sufficient amount of measurements to be statically relevant. The low-resolution data used the same a priori profiles as the TCCON for the processing thereby removing any difference between the datasets due to a priori mismatch.

The current validation results are based on the S-5P and reference measurements available at the time of this analysis, which yield comparison pairs from March 2018 until December 2019. The increased spatial resolution from 7 km to 5.5 km along track since 6 August 2019 (orbit 9388) did not change the performance of the S-5P carbon monoxide product as mentioned in the S5P Mission Performance Centre Quarterly Validation Report (ROCVR #06). Therefore the validation results shown here is for the full time period of the measurements performed between 2018 and 2019 when the FRM4GHG data is also available. Amongst the instrument tested during the FRM4GHG campaign, EM27/SUN and VERTEX70 can provide carbon monoxide and the validation results using the respective datasets are shown here.

5.2.1 S-5P XCO validation using EM27/SUN data

The EM27/SUN performed measurements at the Sodankylä TCCON site during 2017 – 2019.

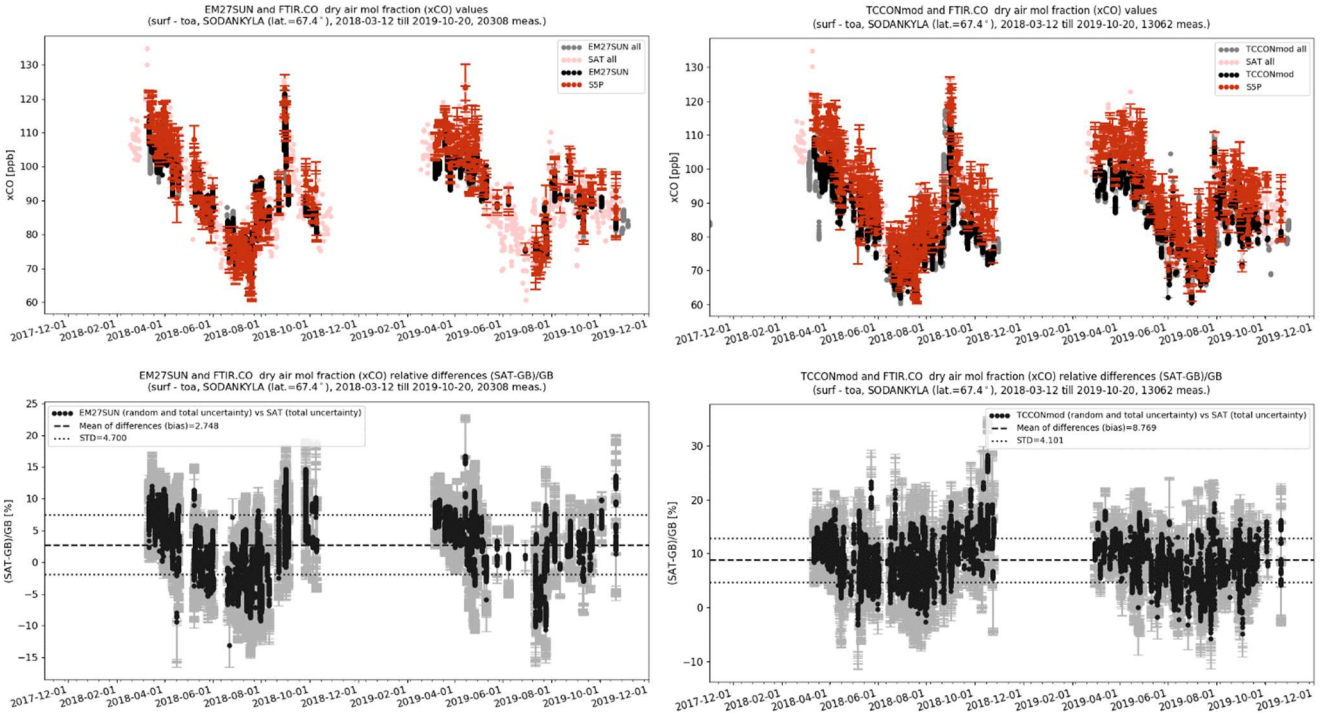

Figure 11: Top-left: Time series of XCO plotted for EM27/SUN (grey) and S-5P (light red) for the year 2018 and 2019. The co-located XCO from EM27/SUN (black) and S-5P (red) are overlaid on the same plot. Top-right: The same plot as the top-left but with TCCON dataset as the reference. Bottom-left: Time series of the XCO relative difference ((SAT – GB)/GB) between the S-5P and EM27/SUN data as reference showing the bias of the S-5P XCO product in relation to the EM27/SUN data. Bottom-right: The same plot as the bottom-left but with TCCON dataset as the reference.

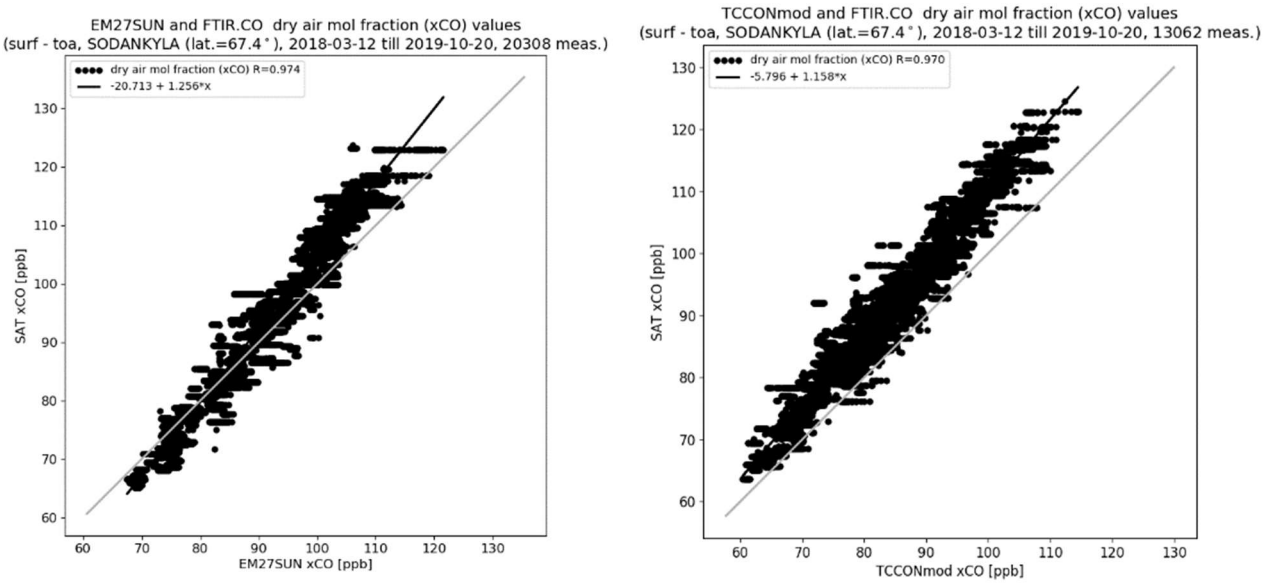

Figure 12: Left: Correlation plot for XCO data between co-located S-5P data and EM27/SUN data for the 2018 – 2019 period. Right: Correlation plot for XCO data between co-located S-5P data and TCCON data for the same period.

The S-5P and EM27/SUN XCO data from the Sodankylä campaign during 2018 and 2019 are plotted in Figure 11. The top figures show the time series with dark red and black points showing the co-located points and error bars showing the scatter in the data. The grey and light-red points show the time series of all measurements. The bottom figures show the XCO relative difference ((SAT – GB)/GB) between the satellite and the reference ground-based instrument. The left panel plots are for S-5P validation results with EM27/SUN data used as the reference ground-based dataset and the right panel plots are with TCCON data used as the reference ground-based dataset. The validation results with the EM27/SUN data show similar patterns as the validation results with the TCCON data. The S-5P is able to capture the seasonal cycle of CO and the high peaks as seen by the reference ground-based FTS instruments. The biases during the spring and autumn period is slightly higher as compared to the bias during the summer period. This feature is seen for both years in 2018 and 2019. The correlation plots of Figure 12 show that the S-5P values are slightly overestimated for high values of XCO in comparison to the ground-based reference datasets. This is due to the differences in the a priori from the true atmospheric state. As the averaging kernel of the instruments are different, the difference of the a priori from the true state will influence the retrieval results differently. The correlation plots shown in Figure 12 for XCO between the S-5P vs EM27/SUN data and those between the S-5P vs TCCON data show similar behaviour and the differences are due to the data representative differences between the EM27/SUN and TCCON datasets.

Table 7: Statistics of S-5P XCO validation using EM27/SUN data and TCCON data as reference from Sodankylä site.

Validation type	Bias %	STD %	R
EM27/SUN vs TCCON	5.55 (5 ppb)	1.37 (1.23 ppb)	0.995
S-5P vs EM27/SUN	2.75	4.7	0.974
S-5P vs TCCON	8.77	4.1	0.970

The EM27/SUN vs TCCON comparison results show a bias of 5.55% with a low scatter of 1.37% and with a high correlation of 0.995. The S-5P vs EM27/SUN validation results show a bias of 2.75% ± 4.7% with a correlation of 0.974. The S-5P vs TCCON validation results show a bias of 8.77% ± 4.1% with a correlation of 0.970. The statistics of the results are shown in Table 7. The bias between the EM27/SUN vs TCCON is also reflected in the bias seen between the S-5P vs EM27/SUN. The results confirm that the bias and the std for S-5P XCO product are compliant with the mission requirement.

5.2.2 S-5P XCO validation using VERTEX70 data

The VERTEX70 performed measurements at the Sodankylä TCCON site during 2017 – 2019.

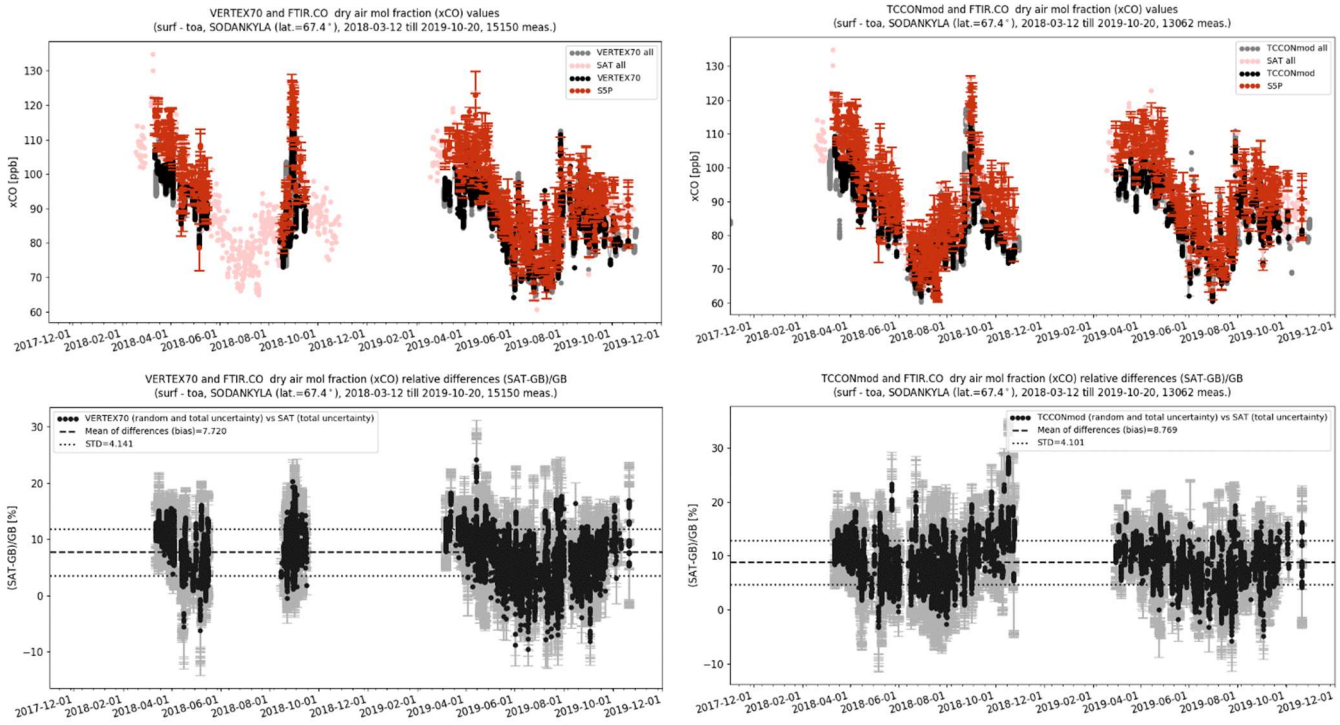

Figure 13: Same plots as Figure 11 but for measurements performed with the VERTEX70 and the TCCON at the Sodankylä site.

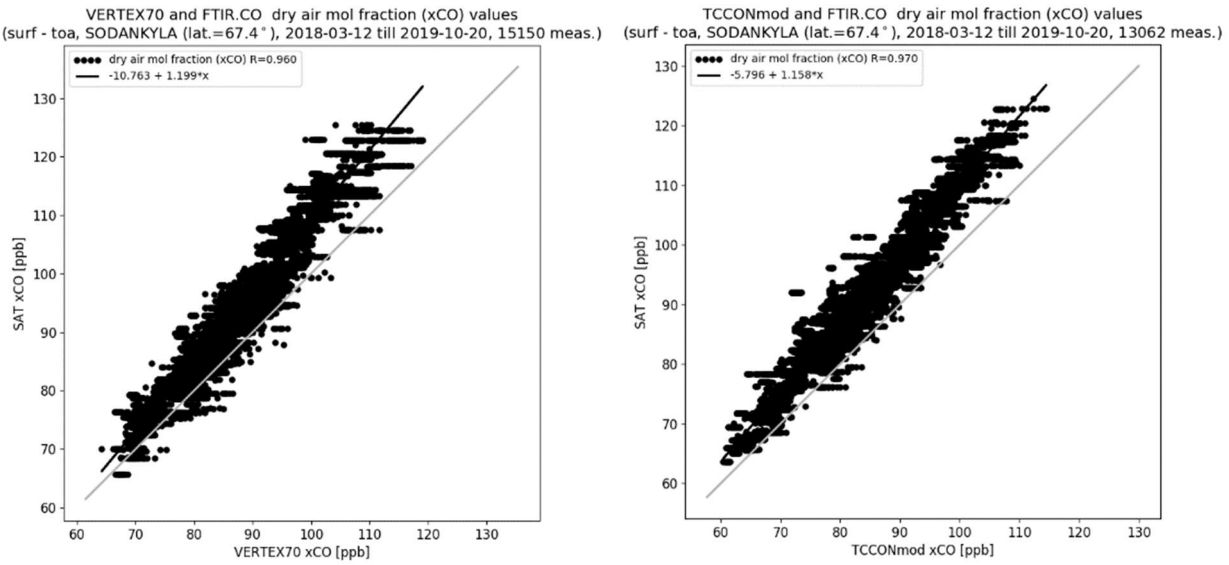

Figure 14: Left: Correlation plot for XCO data between co-located S-5P data and VERTEX70 data for the 2018 – 2019 period. Right: Correlation plot for XCO data between co-located S-5P data and TCCON data for the same period.

The S-5P and VERTEX70 XCO data from the Sodankylä campaign during 2018 and 2019 are plotted in Figure 13. The top figures show the time series with dark red and black points showing the co-located points and error bars showing the scatter in the data. The grey and light-red points show the time series of all measurements. The bottom figures show the XCO relative difference ((SAT – GB)/GB) between the satellite and the reference ground-based instrument. The left panel plots are for S-5P validation results with VERTEX70 data used as the reference ground-based dataset and the right panel plots are with TCCON data used as the reference ground-based dataset. The VERTEX70 instrument has some instrumental modifications to test different detectors in 2018. These measurements are not included, as the results did not show any improvement in comparison to the optimized setting as selected in 2017. The validation results with the VERTEX70 data show similar patterns as the validation results with the TCCON data. The correlation plots of Figure 14 show that the S-5P values are slightly overestimated for high values of XCO in comparison to the ground-based reference datasets. This is similar to what we observe in Figure 12. The correlation plots shown in Figure 14 for XCO between the S-5P vs VERTEX70 data and those between the S-5P vs TCCON data show similar behaviour and the difference are due to the data representative differences between the VERTEX70 and TCCON datasets.

Table 8: Statistics of S-5P XCO validation using VERTEX70 data and TCCON data as reference from the Sodankylä site.

Validation type	Bias %	STD %	R
VERTEX70 vs TCCON	0.77 (0.69 ppb)	0.98 (0.88 ppb)	0.996
S-5P vs VERTEX70	7.72	4.14	0.960
S-5P vs TCCON	8.77	4.1	0.970

The VERTEX70 vs TCCON comparison results show a bias of 0.77% with a low scatter of 0.98% and with a high correlation of 0.996. The S-5P vs VERTEX70 validation results show a bias of 7.72% ± 4.14% with a correlation of 0.960. The S-5P vs TCCON validation results show a bias of 8.77% ± 4.1% with a correlation of 0.970. The statistics of the results are shown in Table 8. The bias between the VERTEX70 vs TCCON is reflected in the bias seen between the S-5P vs VERTEX70. The results confirm that the bias and the std for S-5P XCO product are compliant with the mission requirement.

In this work package, the geophysical validation of S-5P methane and carbon monoxide products above the Sodankylä, Wollongong and Darwin TCCON sites have been addressed based on measurements performed with the low-resolution test instruments and compared to the standard TCCON results. The validation results using the low-resolution instruments showed similar patterns as the validation results using TCCON data. The S-5P methane and carbon monoxide products are fulfilling the mission requirements. The low-resolution instruments EM27/SUN, VERTEX70 and IRCUBE provide measurements of XCO_2, XCH_4 and XCO with high precision and are suitable for being used for satellite validation of these products.

6 Applicable documents

Statement of Work: Fiducial Reference Measurements for Ground-Based FTIR Greenhouse Gas Observations (FRM4GHG)
Prepared by: T. Fehr/B. Bojkov (EOP-GMQ), Reference: ESA-EOPG-MOM-SOW-0007

7 Reference documents

FRM4GHG deliverable D2.5: Validation Plan, made available via the project website
http://frm4ghg.aeronomie.be/index.php/outreach/deliverables

FRM4GHG deliverable D2.4: Data protocol, made available via the project website
http://frm4ghg.aeronomie.be/index.php/outreach/deliverables

S5P Mission Performance Centre Methane [L2__CH4___] Readme
https://sentinel.esa.int/documents/247904/3541451/Sentinel-5P-Methane-Product-Readme-File

S5P Mission Performance Centre Methane [L2__CO___] Readme
https://sentinel.esa.int/documents/247904/3541451/Sentinel-5P-Carbon-Monoxide-Level-2-Product-Readme-File

S5P Mission Performance Centre Quarterly Validation Report of the Copernicus Sentinel-5 Precursor Operational Data Products #01 – #06 http://mpc-vdaf.tropomi.eu/ & http://mpc-vdaf.tropomi.eu/ProjectDir/reports/pdf/S5P-MPC-IASB-ROCVR-06.0.1-20200330_FINAL.pdf

Requirements for the Geophysical Validation of Sentinel-5 Precursor Products
https://earth.esa.int/pi/esa?id=3182&sideExpandedNavigationBoxId=Aos&cmd=image&topSelectedNavigationNodeId=AOS&targetIFramePage=/web/guest/pi-community/apply-for-data/aos&ts=1548864588456&type=file&colorTheme=03&sideNavigationType=AO&table=aotarget

Sentinel-5 Precursor Calibration and Validation Plan for the Operational Phase
https://sentinel.esa.int/documents/247904/2474724/Sentinel-5P-Calibration-and-Validation-Plan.pdf

Sentinel-5 Precursor Scientific Validation Implementation Plan
https://sentinel.esa.int/documents/247904/2474724/Sentinel-5P-Science-Validation-Implementation-Plan

8 Software / tools:

The validation work was performed with the tools developed at BIRA-IASB and written in Python.