S5P MPC VDAF Validation Web Article: Dry air column averaged methane

Contributing authors

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Product definition

The following table contains a description of the S5P TROPOMI processor versions used in this report.

Processor Version	In operation from	In operation until
01.02.02	RPRO orbit 0657, 28-11-2017	RPRO orbit 5346, 25-10-2018
	OFFL orbit 5833, 28-11-2018	present

The OFFL product has the following doi: **http://doi.org/10.5270/S5P-3p6lnwd**

Product requirements are described in the Sentinel-5 Precursor Calibration and Validation Plan for the Operational Phase source: ESA; ref: ESA-EOPG-CSCOP-PL-0073; issue: 1.0 date 2017-06-11, Sentinel-5P-Calibration-and-Validation-Plan.pdf

Validation results

Initial Sentinel-5 Precursor TROPOMI L2_CH_4 dry air averaged methane column data was compared to reference measurements acquired by the FTIR instruments contributing to the NDACC and the TCCON networks. Over the period between November 2017 and December 2018 with the reference data available at the time of this analysis, of the order of 7 NDACC and 23 TCCON stations provided sufficient co-locations sampling sufficient latitudes from the Arctic to the Antarctic. NDACC measurements provide concentration profiles for methane, with sensitivity up to ±20km. TCCON data measure dry air column averaged mole fractions, similar to the TROPOMI product. Because of the different characteristics of the TCCON and NDACC reference data, a slightly different comparison method was used for this validation study as discussed here.

For both NDACC and TCCON type of measurements, averaging kernel data is available which is used to substitute the S5P prior methane profile (available in the L2 product on a per pixel basis) to the FTIR data using the method described in Rodgers (2003). The TCCON measurement (with the S5P prior substituted) is then compared to the S5P XCH_4 column directly since no further reduction of the smoothing error is possible. For NDACC data the method described in Rodgers (2003) is followed one step further and the FTIR CH_4 concentration profile (with the S5P prior substituted) is additionally smoothed with the S5P column averaging kernel.

For the comparisons against NDACC and TCCON the S5P pixel selection criteria were set to a maximal distance of 100 km from the FTIR site and a maximal time difference of 1 hour for TCCON and 3 hours for NDACC. According to the product readme file, pixels were selected to have a qa_value above 0.5.

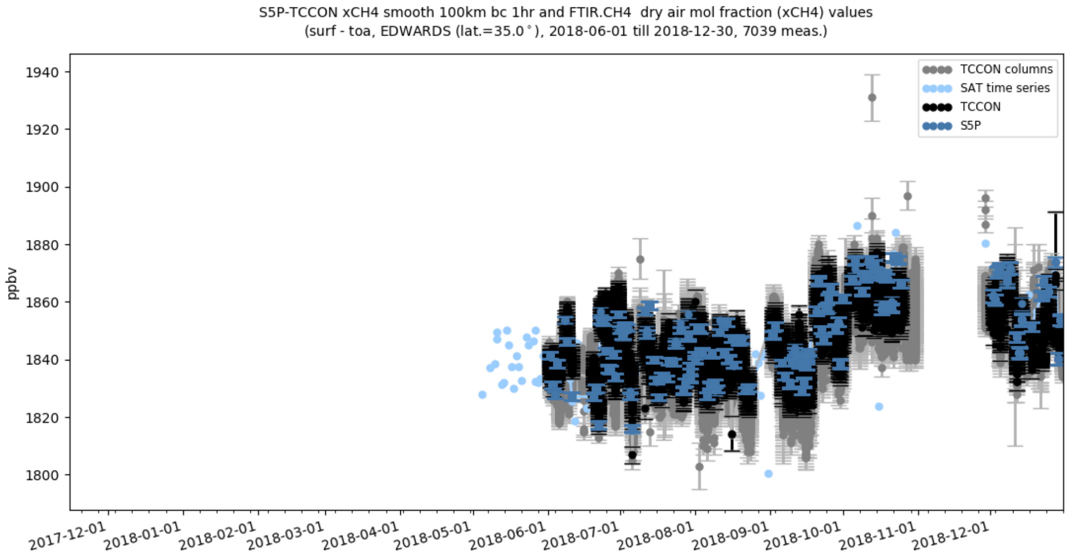

Figure 1 Comparison with TCCON methane measurements at Edwards show that the S5P is able to capture the temporal changes of methane concentration

Ground-based data comparisons lead to the following preliminary conclusions:

- At all of the 23 TCCON and 7 NDACC reference stations, short scale temporal variations in the XCH_4 concentration as captured by ground-based instruments are reproduced very similarly by S5P. Figure 1 illustrates this at the station of Edwards.
- The averaged bias for the comparison against 23 TCCON sites is -0.32% and -0.82% for the bias corrected and standard S5P XCH_4 products. The relative mean difference of the standard XCH_4 product slightly exceeds the mission requirements (bias <1.5%) only at a few TCCON sites (i.e. Sodankylä, East Trout Lake, Parkfalls and Wollongong). However, it never exceeds the mission requirements for the bias corrected product. Figure 2 shows the per station biases for both the bias corrected and standard S5P XCH_4 products. Figure 4 shows the time series of the relative biases.

- The 1σ spread of the relative difference (between the S5P and the TCCON) around the mean value is below the mission requirements (precision <1%) for both the bias corrected and standard products. However, it slightly exceeds above 1% for Kiruna and Sodankylä (see Table 1).
- Compared to the NDACC comparison, TCCON comparisons are statistically more robust and show an averaged correlation of 0.6, see Figure 3. The number of co-locations is too limited in the NDACC comparison to estimate the correlation.

Current conclusions are based on the limited amount of reference measurements available at the time of this first analysis, and on the period covered by the initial S5P dataset (November 2017 to Dec 2018). The current conclusions need to be confirmed by a larger amount of co-locations, and extended over multiple years of data.

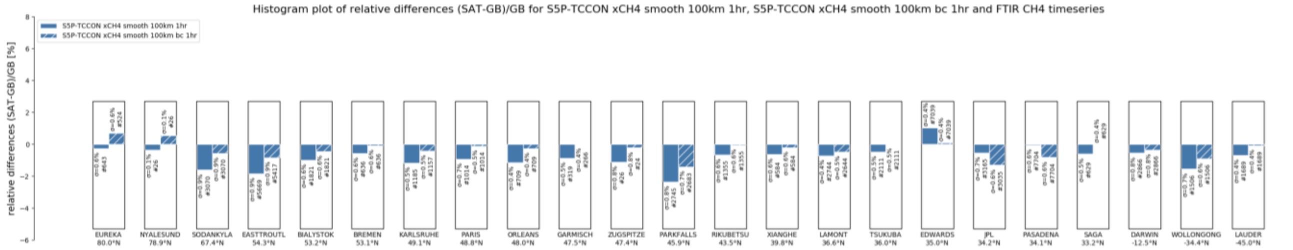

Figure 2 Histogram plot of the relative difference (SAT-GB)/GB in % for the bias corrected (dashed) and standard S5P XCH_4 product for all TCCON stations ordered in decreasing latitude from left to right.

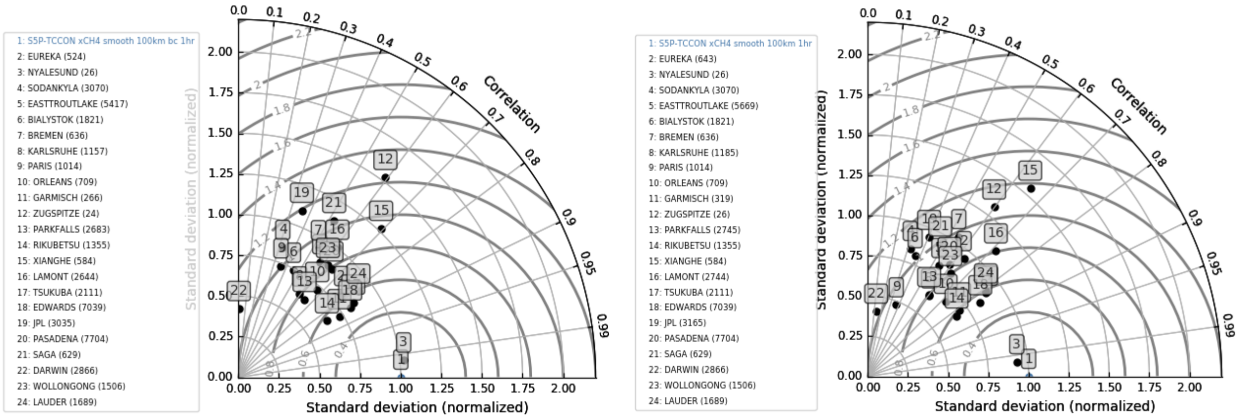

Figure 3 Taylor diagrams for the S5P XCH_4 and ground-based TCCON XCH4 for the standard (left) and bias corrected (right) S5P products. Most stations have a correlation above 0.5. The very low correlation for Darwin is due to the low satellite values for some days. Other stations such as JPL, Paris have limited dataset for the comparison.

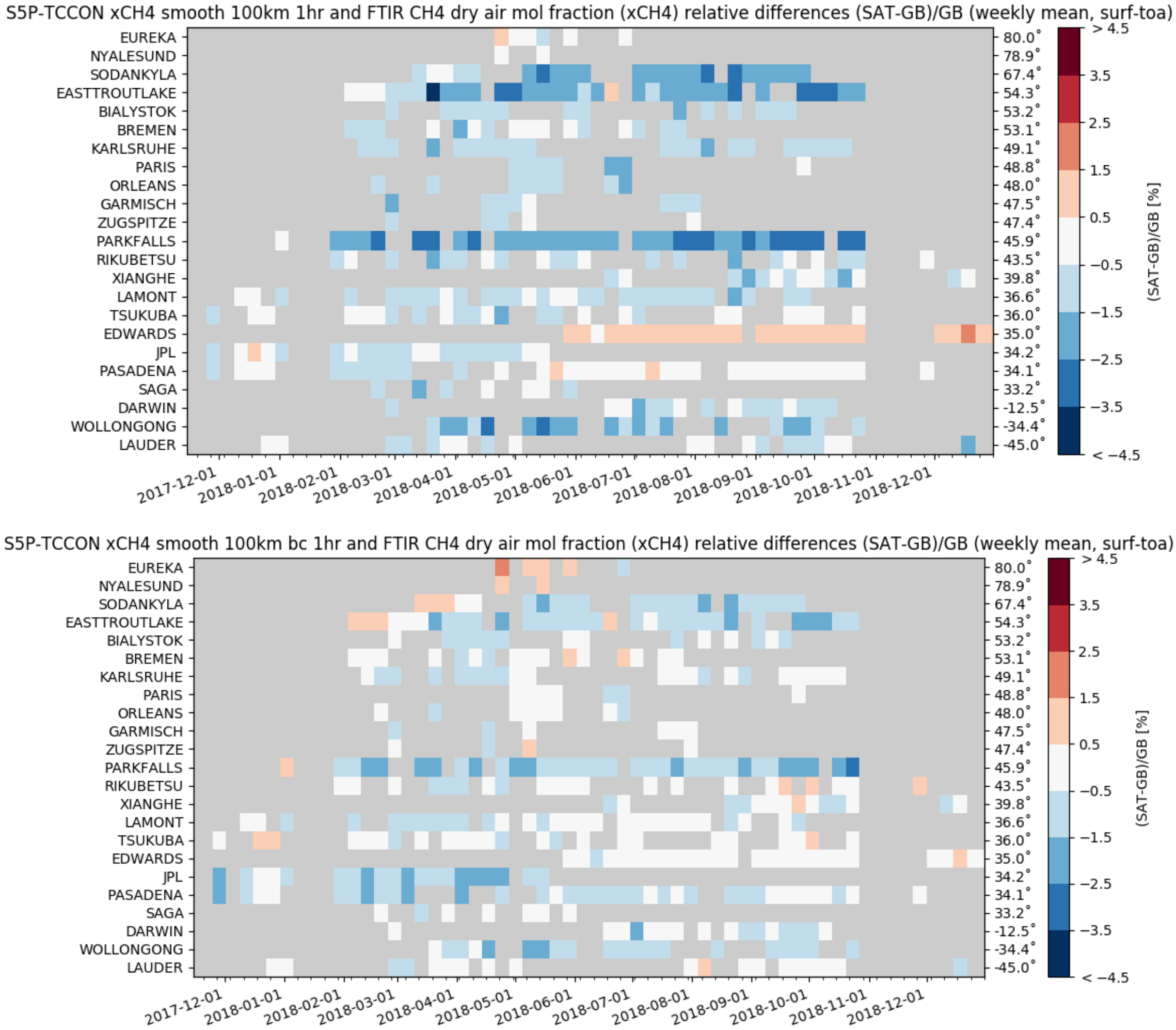

Figure 4 Time series of relative differences for the TCCON stations (top standard S5P product, bottom is bias corrected S5P product). Although the time period is limited, the biases seem stable throughout the year. At the higher latitude stations a change in sign is observed during the spring months (bottom plot).

NDACC site	# days	Std	correlation	rel diff bias(%)	rel diff std(%)	lat
EUREKA	22	0.9	0.55	-0.42	0.60	80.1
KIRUNA	45	1.1	0.09	-0.96	1.30	67.8
SODANKYLA	57	1.0	0.02	-0.68	1.17	67.4
ST.PETERSBURG	50	1.1	0.32	-0.70	0.96	59.9
BREMEN	13	0.8	0.78	0.91	0.47	53.1
JUNGFRAUJOCH	9	0.9	0.77	-0.39	0.43	46.6
LAUDER	20	1.3	0.76	0.17	0.61	-45.0
Mean values for standard product		1.0	0.47	-0.29	0.79	

NDACC site	# days	Std	correlation	rel diff bias(%)	rel diff std(%)	lat
EUREKA	22	0.8	0.44	0.33	0.70	80.1
KIRUNA	45	1.0	0.10	0.03	1.37	67.8
SODANKYLA	57	1.0	0.06	0.36	1.16	67.4
ST.PETERSBURG	50	1.1	0.46	0.28	0.86	59.9
BREMEN	13	0.9	0.74	1.46	0.49	53.1
JUNGFRAUJOCH	9	0.9	0.77	0.27	0.43	46.6
LAUDER	20	1.3	0.80	0.76	0.58	-45.0
Mean values for bias corrected product		1.0	0.48	0.50	0.80	

Table 1: Overview of the relative biases for the NDACC instruments.

Known data issues

Currently, the following data quality issues are known, not covered by the quality flags, and should be kept in mind when looking at the methane product and also at preliminary validation results.

- Filtering on qa value >0.5 does not remove all pixels considered bad. Some pixels with too low and too high methane concentrations are still present, see Figure 4
- Single TROPOMI overpasses show stripes of erroneous CH_4 values in the flight direction, see Figure 6 (left)
- Not all pixels above inland water are filtered with the qa_value flag, see Figure 6 (right)
- Uncertainties for the XCH_4 are only based on the single sounding precision due to measurement noise. For applications requiring an overall uncertainty estimate, we propose to multiply the provided error by a factor 2, which reflects the scatter of single sounding errors in the TCCON validation.
- The current data release only provides XCH_4 over land. Glint ocean observations will be added in the next data release.

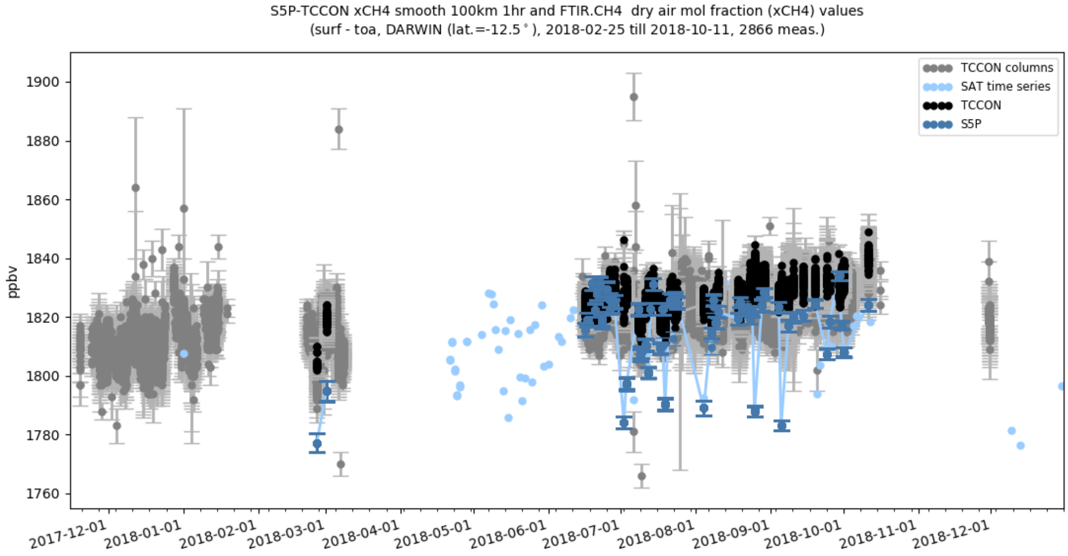

Figure 5 S5P XCH_4 time series over Darwin where low values of XCH_4 are observed for several days.

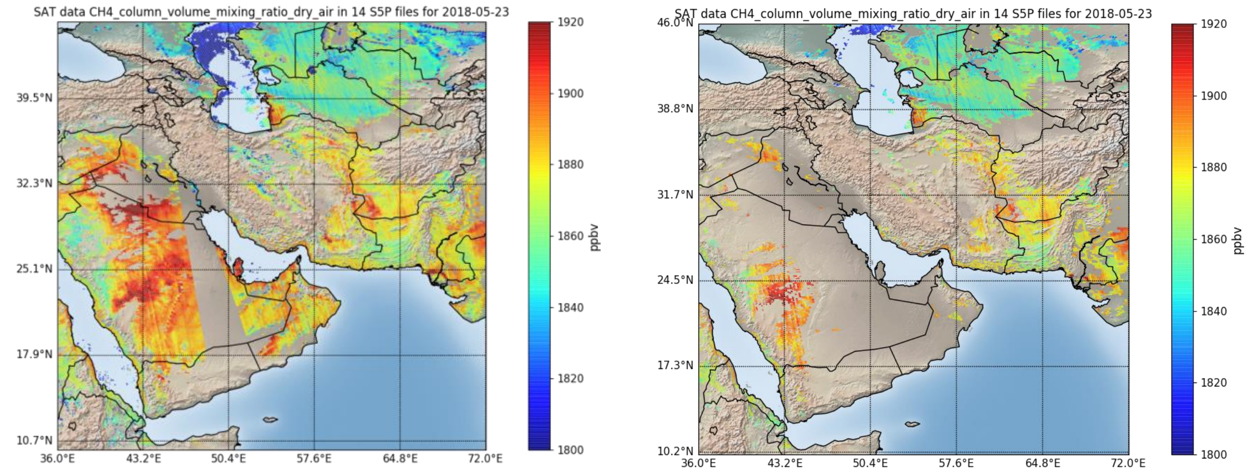

Figure 6 Maps showing XCH_4 concentrations above the Middle East measured on May 23 2018. The left panel shows all available pixels, the right panel shows only pixels with qa_value>0.5. The left panel shows the presence of stripes in the flight direction and the right panel shows the presence of filtered pixels above inland water (Caspian Sea).

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