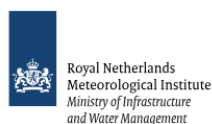




# S5P Mission Performance Centre Methane [L2\_\_CH4\_\_\_] Readme



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<sup>1</sup> The S5PVT AO project summaries can be found at <https://earth.esa.int/web/guest/pi-community/search-results-and-projects/mission>

## CHANGE LOG

Reason for change	Issue	Revision	Date
Cloud mask is based on VIIRS ECM product (instead for VICMO) since orbit 12432 (see section 4.3)	1	4	11/03/2020

## 1 Summary

This is the Product Readme File (PRF) for the Sentinel 5 Precursor Tropospheric Monitoring Instrument (S5P/TROPOMI) Methane (CH<sub>4</sub>) total column level 2 data product and is applicable for the Offline (OFFL) timeliness data product.

A change in the Copernicus Sentinel 5P operations scenario, towards an increased spatial resolution from 7.0 km to 5.5 km along track for all measurements, became operational starting from 6 August 2019, orbit 9388.

Product Identifier: **L2\_\_CH4\_\_**

Example filename:

**S5P\_OFFL\_L2\_\_CH4\_\_20190115T172935\_20190115T191105\_06517\_01\_010202\_20190121T194108.nc**

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

The Readme file describes the current processing baseline, product and quality limitations, and product availability status. More information on this data product is available from the Copernicus Sentinel product webpage:

<https://sentinels.copernicus.eu/web/sentinel/technical-guides/sentinel-5p/products-algorithms>,

and from the TROPOMI product webpage <http://www.tropomi.eu/data-products>.

The data file contains the column average dry air mixing ratio of methane, XCH<sub>4</sub> (`methane_mixing_ratio`), which gives the total atmospheric column between the surface and the top of the atmosphere normalized to the corresponding dry air column. The respective random error originating from the spectral fit is given in the methane (CH<sub>4</sub>) total column `_precision`. As a user guideline for the data quality a `qa_value` is given with the data. In order to avoid misinterpretation of the data quality, it is recommended at the current stage to only use those pixels with a `qa_value` above 0.5.

Independent validation by S5p Mission Performance Centre (MPC) Cal/Val experts and the Sentinel-5 Precursor Validation Team (S5PVT) concludes that the methane total column data is in good overall agreement with (i) reference measurements collected from the TCCON and NDACC global ground-based networks, and (ii) the corresponding satellite data products from GOSAT.

An overall bias of -0.3% (-0.8% for `methane_mixing_ratio_not_bias_corrected`) is found in the MPC Validation Data Analysis Facility (VDAF) data comparison against 22 TCCON stations and is well within the mission requirements (Table 1) of  $\leq 1.5\%$  (24 ppb). The scatter of the data around this bias also complies with mission requirements of  $\leq 1.0\%$  (18 ppb). The comparison of S5p TROPOMI and GOSAT XCH<sub>4</sub> product supports the findings of the data product validation with ground-based measurements.

**The data product requirements are listed in the S5p Calibration and Validation Plan [RD01]**

Parameter	Data product	Vertical Resolution	Bias	Random
Total column OFFL	Methane (CH <sub>4</sub> )	Total column	1.5%	1.0%

Table 1: Mission data requirements for the CH<sub>4</sub>

## 2 Processing baseline description

The Table 2 contains the history of the CH<sub>4</sub> processor versions.

Also reprocessed CH<sub>4</sub> data products ('RPRO' tag in filename) have been made available on the Copernicus Sentinel-5P Pre-operations Data Hub. The 'RPRO' products that are available with version 01.02.02 for selected orbits (list available here <https://sentinels.copernicus.eu/documents/247904/2474724/Reprocessed-S5p-CH4-orbit-list-1.0.pdf>) were processed in the frame of the Validation campaign performed prior to the public CH<sub>4</sub> data release. After the public data release, the remaining products in the period between orbit 2818 (2018-04-30) - Orbit 5832 (2018-11-28) were reprocessed (with version 01.03.01).

Note that the processor version for CH<sub>4</sub> is changing when there is a change to any of the products belonging to the NL-L2 processor suite (NO<sub>2</sub>, CO, CH<sub>4</sub>, AI, ALH, O<sub>3</sub> PR) even if the change is not affecting the CH<sub>4</sub> product.

Processor Version	In operation from	In operation until	Relevant improvements
01.03.02	OFFL: orbit 8815, 2019-06-26	Current version	No changes with respect to previous version
01.03.01	RPRO: orbit 2818, 2018-04-30 OFFL: orbit 7907, 2019-04-23	Orbit 5832, 2018-11-28 Orbit 8814, 2019-06-26	Reprocessed to fill the gaps left during the reprocessing with V01.02.02 No changes with respect to previous version
01.03.00	OFFL: orbit 7425, 2019-03-20	Orbit 7906, 2019-04-23	Added new variables: <code>eastward_wind</code> and <code>northward_wind</code>
01.02.02	RPRO: orbit 2830, 2018-04-30 OFFL: orbit 5833, 2018-11-28	Orbit 5346, 2018-10-25 Orbit 7424, 2019-03-20	Reprocessed for selected orbits Initial operational version

Table 2: History of CH<sub>4</sub> processor versions.

## 3 Product Quality

### 3.1 Recommendations for data usage

It is recommended to use TROPOMI CH<sub>4</sub> data associated with a quality assurance value `qa_value` > 0.5. The `qa_value` is provided as part of the CH<sub>4</sub> data product and the overall definition used in the current data release is summarized in Table 3. A more detailed discussion on the `qa_value` parameter can be found in the Algorithm Theoretical Basis Document (ATBD) [RD02].

<code>qa_value</code>	Condition	Remark
1.0	Convergence, clear-sky	Highest quality data
0.8	Failed deconvolution irradiance spectrum	Not pixel specific but row-specific
0.4	<ul style="list-style-type: none"> <li>Not confidentially clear-sky (VIIRS, non-scattering retrieval)</li> <li>SZA &gt; 70°, VZA &gt; 60°</li> <li>Surface albedo (SWIR) &lt; 0.02</li> <li>Fraction of 'good' spectral pixels (SIWR, NIR) &lt; 70%</li> <li>AOT &lt; 0.3,</li> <li>CH<sub>4</sub> noise related error &lt; 10</li> <li><math>\chi^2</math> &lt; 100</li> <li>SNR SWIR &lt; 50</li> </ul>	<p>For details in cloud filter see Sect. 5.4 of the ATBD [RD02]</p> <p>Thresholds are specified in configuration file</p>
0.0	No convergence	

Table 3: `qa_value` definition

Current TROPOMI CH<sub>4</sub> data is available only for inner 2/3 of the swath (VZA < 60°) and over land.

For further details, data users are encouraged to read the Product User Manual (PUM) [RD03] and ATBD [RD02] associated with this data product, both available on <https://sentinels.copernicus.eu/web/sentinel/technical-guides/sentinel-5p/products-algorithms>.

### 3.2 Validation results

#### 3.2.1 Status of product validation

This section presents a summary of the key validation results obtained by VDAF of the S5p MPC and by the S5PVT activities. Current conclusions are based on the limited amount of reference measurements available at the time of this analysis, and on the period covered by the initial S5p dataset. The conclusions summarized hereafter need to be confirmed by a larger amount of co-locations, and extended over multiple years of data, hence, a full cycle of key influence quantities, in order to enable detection and quantification of potential patterns, dependences, seasonal cycles and longer-term features.

### 3.2.2 Validation approach

#### 3.2.2.1 Ground-based networks

S5P/TROPOMI L2\_\_CH4\_\_ methane total column data are routinely compared to reference measurements of the TCCON and NDACC networks.

#### 3.2.2.2 Satellites

Initial S5P/TROPOMI L2\_\_CH4\_\_ methane total column data have also been compared to GOSAT CH<sub>4</sub> data (Hu et al., 2018).

#### 3.2.2.3 Model

Not done yet

### 3.2.3 Validation results

Hu et al., 2018 [RD04] compared the column averaged dry air mole fraction of methane (XCH<sub>4</sub>) with spatiotemporal collocated XCH<sub>4</sub> measurements of the Japanese GOSAT mission. For intercomparing TROPOMI and GOSAT methane observations, they chose the methane proxy product, that is delivered in the context of the Copernicus Atmospheric Monitoring Service (CAMS, [RD05]). The proxy approach uses radiance measurements in the 1.6  $\mu$ m spectral range covering weak absorption bands of CO<sub>2</sub> and CH<sub>4</sub>. The method infers the total column density of both trace gases [CH<sub>4</sub>] and [CO<sub>2</sub>] ignoring any atmospheric scattering and relies on the assumption that scattering effects cancel in the ratio of the CH<sub>4</sub> column [CH<sub>4</sub>] and the CO<sub>2</sub> column [CO<sub>2</sub>], and that a prior estimate of XCO<sub>2</sub> is sufficiently accurate to recalculate the XCH<sub>4</sub> from the measured [CH<sub>4</sub>]/[CO<sub>2</sub>] ratio [RD07]. The GOSAT data product is bias-corrected with respect to high-precision ground-based measurements from the TCCON [RD06] but has a remaining bias of -6.6 ppb and a standard deviation of 15.5 ppb with respect to TCCON measurements. Note that the proxy method cannot be applied to TROPOMI measurements, because there is no suitable light-path proxy for CH<sub>4</sub> in the 2.3  $\mu$ m band and so this comparison relies not on two different spectrometers but also on different retrieval methods and two different spectral ranges.

Using TROPOMI measurements with the 2-band operational retrieval algorithm [RD08] from 11 November to September 2018 and following the comparison approach in Hu et al., 2018, we find a very good agreement between TROPOMI and GOSAT methane products with a mean difference of 7.4 ppb, a standard deviation of 21.0 ppb, and a Pearson's correlation coefficient of 0.86.

The inspection of the GOSAT and TROPOMI product indicated a clear albedo dependence of the differences between both data product with a clear underestimation of the TROPOMI XCH<sub>4</sub> data for low albedo. Based on this, a bias correction is derived and applied to the current version of the data product (see for more details the product ATBD [RD02]), leading to the bias-corrected XCH<sub>4</sub> entry (`methane_mixing_ratio_bias_corrected`) of the TROPOMI data product.

As part of the S5PVT activity 'Validation of the S5p CO and CH<sub>4</sub> total column product' (AO Proposal ID28630), preliminary validation has been performed by SRON of a (re) processed subset of S5p TROPOMI CH<sub>4</sub> clear-sky measurements retrieved over TCCON stations. For this validation, we used independent ground based CH<sub>4</sub> measurements from 12 different stations located in North America, Asia, Europe and Oceania. We selected TROPOMI measurements from the same day as the TCCON measurements within a radius of 300 km around each station and found an agreement between TROPOMI CH<sub>4</sub> and TCCON of -12 ppb, with a station-to-station variability (i.e. standard deviation of the mean bias for all stations) of 11.5 ppb. If the radius is reduced to 50 km, the bias is -13.6 ppb, but the number of co-located measurements is reduced by 60%. The agreement between TROPOMI CH<sub>4</sub> corrected for the albedo dependency (see ATBD [RD02]) and TCCON (for a collocation radius of 300 km) is of -4.3 ppb, with a station-to-station variability of 7.4 ppb. The comparison results show that the quality of the TROPOMI CH<sub>4</sub> and CH<sub>4</sub> corrected product is such that they both largely comply with the mission requirements specified in Table 1.

The S5p MPC VDAF and the TCCON4S5P AO project performed a validation against all data available in both TCCON and NDACC networks covering the period 11/2017 – 12/2018 for both the standard XCH<sub>4</sub> S5p data product and the bias corrected product. The validation methodology compares the groundbased column with the satellite column after substitution of a common prior (see Rodgers et. al 2003, the S5p prior is used as the common prior). For the comparison against TCCON the S5p pixel selection criteria were set to a maximal distance of 100km from the FTIR site and a maximal time difference of 1 hour. Validation results show that both the S5p standard and bias corrected XCH<sub>4</sub> products satisfy the mission requirements. The comparison against TCCON leads to the following conclusions:

- The averaged bias for the comparison against 22 TCCON sites is -0.81% and -0.31% for the standard and bias corrected XCH<sub>4</sub> product. The relative mean difference of the standard XCH<sub>4</sub> product slightly exceeds the mission requirements (bias <1.5%) only at a few TCCON sites (e.g. Sodankylä, Easttroutlake, Parkfalls and Wollongong).
- The network wide average of the standard deviations of the relative differences is estimated at 0.6% for both standard and bias corrected products and lies well within the mission requirement on precision (<1%). All TCCON sites estimate the S5p precision below the required 1%.

For more details validation results, the user is referred to the S5p MPC VDAF website at <http://mpc-vdaf.tropomi.eu> and [RD04].

We thank all the TCCON and NDACC PI's for providing the data without which this validation study would not have been possible.



## 4 Data Quality Remarks

### 4.1 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. For more details we refer to the MPC VDAF website <http://mpc-vdaf.tropomi.eu>.

#### Variable `qa_value`

Filtering on `qa_value` > 0.5 does not remove all pixels considered bad. Some pixels with too low methane concentrations are still present.

#### Stripes

Single TROPOMI overpasses show stripes of erroneous CH<sub>4</sub> values in the flight direction.

#### Uncertainties estimation

Uncertainties for the XCH<sub>4</sub> 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.

#### Data only over land

The current data release only provides XCH<sub>4</sub> over land. Glint ocean observations will be added in the next data release.

#### Metadata/Attributes

The spatial resolution of the TROPOMI measurements is improved by bringing the along track ground pixel size from 7.0 to 5.5 Km starting on 6<sup>th</sup> August 2019. Note that, after this operations change, the metadata/Attributes fields listed below related to the spatial resolution, remain **unchanged** (hence not aligned to the improved resolution). These fields are planned to be updated with the activation of Level 2 processors version 02.xx.xx by the beginning of 2020.

### 4.2 Solved Data Quality Issues

#### Inland water pixels (solved)

Not all pixels above inland water are filtered. This is solved since orbit **7644 (05-APR-2019)**.

### 4.3 Data Features

This section describes some characteristics of the data that might seem anomalous, however they are physically correct and not related to any problem.

#### Pixel geolocation around North Pole

The solar irradiance is measured on a daily basis over the North Pole at a reference azimuth angle to remove seasonal effects on the measurements. To this end, a yaw manoeuvre is executed when the instrument is still in radiance mode, causing possible distortion on the scanlines observed during this manoeuvre (i.e. crossing scanlines, "bow-tie" ground pixel shape instead of rectangular). This occurs at most during the last 26 seconds of radiance measurements in few orbits (7-9 per week). Though this may seem anomalous, it is physically correct, and not related to any problem on the data geolocation.

### **New cloud mask for S-NPP used during CH4 processing**

NOAA no longer supports the VIIRS cloud mask (VCM or VICMO) product, which is discontinued (second quarter 2020) in favour of the Enterprise Cloud Mask (ECM). An update to the S5P-NPP L2 processor (to version 01.01.00) has happened (orbit 12432, date 07-03-2020) to ingest the new cloud mask. It should, however, be noted that there are significant differences between the cloud mask fields themselves: E.g. compared to VCM, ECM tends to indicate fewer confidently clear scenes over land, but more over sea. Therefore, values in the cloud/clear counts used to calculate the cloud fraction for the filtering of the CH4 product are now different.

The change in cloud fractions (sign and magnitude) are dependent on the day and location. However, the current thresholds for cloud filtering do not affect the CH4 product, i.e. cloudy scenes are filtered properly. Full assessment of data quality will come after the new processor has been running long enough.

## **5      Algorithm Change Record**

For a detailed description of the L2\_\_CH4\_\_ algorithms, please refer to the ATBD [RD02].

## **6 Data Format**

The product is stored as NetCDF4 file. The NetCDF4 file contains both the data and the metadata for the product.

Details of the data format are provided in the PUM document [RD03].

### **6.1 Data format changes**

#### **Version 01.03.00**

- The fields "eastward\_wind" and "northward\_wind" are added to the L2 files.

## 7 Product Availability

S5P/TROPOMI Methane data are available on the Copernicus S5p Open Access Hub <https://scihub.copernicus.eu/>

More information on this data product and data handling tools are available from the product web page under heading 'Tools': <http://www.tropomi.eu/data-products>.

For further questions regarding S5P/TROPOMI data products please contact [EOSupport@Copernicus.esa.int](mailto:EOSupport@Copernicus.esa.int).

The access and use of any Copernicus Sentinel data available through the Copernicus Sentinel Data Hub is governed by the Legal Notice on the use of Copernicus Sentinel Data and Service Information and is given here:

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## 8 References

- [RD01] Sentinel-5 Precursor Calibration and Validation Plan for the Operational Phase  
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url: <https://sentinel.esa.int/documents/247904/2474724/Sentinel-5P-Calibration-and-Validation-Plan.pdf>
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More information on this data product is available from the Copernicus Sentinel product webpage:

<https://sentinels.copernicus.eu/web/sentinel/technical-guides/sentinel-5p/products-algorithms>,

and from the corresponding TROPOMI product webpage <http://www.tropomi.eu/data-products>.

## Abbreviations and acronyms

ATBD	Algorithm Theoretical Basis Document
BIRA-IASB	Royal Belgian Institute for Space Aeronomy
CAMS	Copernicus Atmosphere Monitoring Service
CH <sub>4</sub>	Methane
ECM	Enterprise Cloud Mask
ESA	European Space Agency
ESL	Expert Support Laboratory
ESRIN	European Space Research Institute
FTIR	Fourier Transform Infra-Red
IFS	ECMWF Integrated Forecasting System
KNMI	Royal Netherlands Meteorological Institute / Koninklijk Nederlands Meteorologisch Instituut
MOPITT	Measurements of Pollution in the Troposphere
MPC	Mission Performance Centre
NDACC	Network for the Detection of Atmospheric Composition Change
OFFL	Offline
PRF	Product Readme File
PUM	Product User Manual
RPRO	Reprocessing
S5P	Sentinel-5 Precursor
S5PVT	Sentinel-5 Precursor Validation Team
SZA	Solar Zenith Angle
TCCON	Total Carbon Column Observing Network
TROPOMI	TROPOspheric Monitoring Instrument
VCM	VIIRS Cloud Mask
VDAF	Validation Data Analysis Facility
VZA	Viewing Zenith Angle