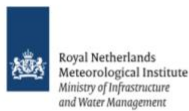




S5P Mission Performance Centre Methane [L2__CH4___] Readme



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¹ The S5PVT AO project summaries can be found at
<https://earth.esa.int/eogateway/news/announcement-of-opportunity-for-s5pvt>

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
Table 2: addition of version 01.04.00 Section 4.1: addition of the "Less valid CH ₄ data since the activation of VIIRS ECM" paragraph	1	5	11/12/2020
Table 2: Adapting to V02.02.00 of the processor Section 3.2: Validation results shortened, pointing to the routine Validation reports Section 4.1 & section 4.2: some text moved from section 4.1 (Known Data Issues) to section 4.2 (Solved Data Quality Issues) Section 6.1: added format changes related to version 02.02.00	2	0	05/07/2021
Table 2: addition of version 02.03.01 Section 4.1 & section 4.2: some text moved from section 4.1 (Known Data Issues) to section 4.2 (Solved Data Quality Issues) Section 6.1: added minor format changes related to version 02.03.01	2	1	17/11/2021

1 Summary

This is the Product Readme File (PRF) for the Sentinel 5 Precursor Tropospheric Monitoring Instrument (S5P/TROPOMI) Methane (CH₄) total column level 2 data product and is applicable for the Offline (OFFL) timeliness data product.

Product Identifier: **L2_CH4**

Example filename:

S5P_OFFL_L2_CH4_20210913T001559_20210913T015729_20297_02_020200_20210914T165118.nc

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

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, XCH₄ (`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. It also contains the data corrected for the XCH₄ dependence on surface albedo (`methane_mixing_ratio_bias_corrected`). More information on the a-posteriori correction can be found in the Algorithm Theoretical Basis Document (ATBD) [RD02]. The respective random error originating from the spectral fit is given in the methane (CH₄) 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.

Note: Starting from processor version 2.2.0, new improved Level 1b version 2.0 data products are used as input [RD05].

In addition, starting from processor version 2.3.1 the retrieval of methane data over ocean sun glint areas has been introduced.

Independent validation by S5p Mission Performance Centre (MPC) Cal/Val experts and the Sentinel-5 Precursor Validation Team (S5PVT) concludes that the version 1.x.x of the methane total column data is compliant with the requirements as defined in the **S5P Calibration and Validation Plan** [RD01], see Table 1.

Up to date validation results are available in the Routine Operations Consolidated Validation Reports (ROCVR) that are accessible through the MPC Validation Data Analysis Facility (VDAF) website at <http://mpc-vdaf.tropomi.eu>. The ROCVR reports are issued quarterly, and reports released after September 2021 include validation results based on processor version 2.x.x.

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 ₄)	Total column	1.5%	1.0%

Table 1: Mission data requirements for the CH₄

2 Processing baseline description

The Table 2 contains the history of the CH₄ processor versions. Reprocessed CH₄ data products ('RPRO' tag in filename) have been also 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 CH₄ 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 CH₄ is changing when there is a change to any of the products belonging to the NL-L2 processor suite (NO₂, CO, CH₄, AI, ALH, O₃ PR) even if the change is not affecting the CH₄ product.

Processor Version	In operation from	In operation until	Relevant improvements
02.03.01	OFFL: orbit 21188, 2021-11-14	Current version	<ul style="list-style-type: none"> Retrieval of methane data over ocean sun glint areas Minor changes in format (see section 6.1)
02.02.00	OFFL: orbit 19258, 2021-07-01	Orbit 21187, 2021-11-14	<ul style="list-style-type: none"> Update CH₄, CO and H₂O cross sections in the CO and CH₄ processors: the updated cross sections are based on DLR Scientific Exploitation of Operational Missions – Improved Atmospheric Spectroscopy Databases (SEOM-IAS) spectroscopy (https://zenodo.org/record/1009126#.YJurduvRaL4) The a-posteriori bias corrected CH₄ is now independent of any reference data (in the operational algorithm version 1.x.x, a correction based on the comparison of TROPOMI XCH₄ with GOSAT retrievals was applied) Changes in format (see section 6.1) <p>Note: Starting from processor version 2.2.0, a new improved Level 1b version 2.0 data products are used as input [RD05]</p>
01.04.00	OFFL: orbit 16213, 2020-11-29	Orbit 19257, 2021-07-01	No changes with respect to previous version
01.03.02	OFFL: orbit 8815, 2019-06-26	Orbit 16212, 2020-11-29	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 CH₄ processor versions.

3 Product Quality

3.1 Recommendations for data usage

It is recommended to use TROPOMI CH₄ bias corrected data (`methane_mixing_ratio_bias_corrected`) associated with a quality assurance value `qa_value` > 0.5. The `qa_value` is provided as part of the CH₄ 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].

qa_value	Condition	Remark
1.0	Convergence, clear-sky	Highest quality data Contains both land and ocean data
0.8	Failed deconvolution irradiance spectrum	Not pixel specific but row-specific
0.4	<ul style="list-style-type: none"> • Not confidentially clear-sky (VIIRS, non-scattering retrieval as back-up) • SZA > 70° • Surface albedo (SWIR) < 0.02 • AOT (NIR) > 0.3, • CH₄ noise related error > 10 • $\chi^2 > 100$ • Terrain roughness > 80 	For details in cloud filter see Sect. 5.4 of the ATBD [RD02] Thresholds are specified in configuration file
0.0	No convergence or Pre-filter: <ul style="list-style-type: none"> • Cloud fraction > 0.02 • Terrain roughness > 100 m • SZA > 75°, VZA > 60° • Fraction of 'good' spectral pixels (SIWR, NIR) < 70% • SNR SWIR > 50 	

Table 3: `qa_value` definition

Applying the recommended `qa_value` > 0.5 includes, since version 2.3.1, pixels both over land and over ocean. If users want to use only land or ocean pixels, they should include in their filtering the `processing_quality_flags` or `surface_classification` mask to select pixels with `sun_glint_warning` and `water` flag.

Current TROPOMI CH₄ data is available only for inner 2/3 of the swath (VZA < 60°).

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

Independent validation by S5p Mission Performance Centre (MPC) Cal/Val experts and the Sentinel-5 Precursor Validation Team (S5PVT) concludes that the version 1.x.x of 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. In particular, an overall bias of -0.3% (-0.7% for `methane_mixing_ratio` without the bias correction) is found in the MPC Validation Data Analysis Facility (VDAF) data comparison against 28 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) [RD04]. The comparison of S5p TROPOMI and GOSAT XCH₄ product supports the findings of the data product validation with ground-based measurements.

The quality of the processor version 2.x.x has been assessed on a dedicated Test Data Set of roughly 2 weeks with the expected results (better data coverage due to the cloud fraction definition modification to include the 'probably clear' pixels, and improved overall quality of spectral fit of the retrieval due to the updated spectroscopy).

Up to date validation results are available in the Routine Operations Consolidated Validation Reports (ROCVR) that are accessible through the MPC Validation Data Analysis Facility (VDAF) website at <http://mpc-vdaf.tropomi.eu>. The ROCVR reports are issued quarterly, and reports released after September 2021 include validation results based on processor version 2.x.x.

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

4 Data Quality Remarks

4.1 Known Data Quality 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 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 CH₄ values in the flight direction.

Uncertainties estimation

Uncertainties for the XCH₄ 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.

4.2 Solved Data Quality Issues

Inland water pixels (solved)

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

Metadata/Attributes (solved in version 02.02.00)

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 6th August 2019. Note that, after this operations change, the metadata/Attributes fields related to the spatial resolution, remained **unchanged** (hence not aligned to the improved resolution). These fields have been updated with the activation of Level 2 processor version 02.02.00.

Less valid CH₄ data since activation of VIIRS Enterprise Cloud Mask (ECM) on March 2020 (solved in version 02.02.00)

The change in sign and magnitude of the cloud fractions between VIIRS Cloud Mask (VCM) and Enterprise Cloud Mask (ECM) algorithms (see section 4.3) are dependent on the day and location, however cloudy scenes are quite well identified and filtered. Nevertheless, it has been observed that current cloud filtering thresholds are too stringent causing a decrease of around 30% of the number of valid CH₄ measurements since the activation of the ECM data usage. It is to be noted that from September 2020 this problem is much less evident. Full assessment of data quality has been performed and improved cloud filtering has been implemented within version 02.02.00.

No CH₄ data produced when VIIRS input data was not available (solved in version 02.03.01)

In version 02.02.00, the production of CH₄ was failing if no VIIRS input data were available. This has been solved in version 02.03.01.

Data only over land (solved in version 02.03.01)

The data released before version 02.03.01 only provided XCH₄ over land. Glint ocean observations were added in the data release of version 02.03.01.

Geolocation co-added when they should not be (solved in version 02.03.01)

In version 02.02.00, the geolocation of pixels near the pole show a shift of up to 300 meters due to a co-addition activity performed by mistake. This has been corrected in version 02.03.01.

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.

Negative surface albedo over ocean

The retrieved surface albedo over ocean for sun-glint measurements might be lower than zero (i.e., negative values). This is because ocean measurements use a different reflectance model than that over land. Therefore, retrieved surface albedo over ocean does not have the same physical meaning as that over land.

Solar zenith angle cycle

To assure the highest quality of the data, a filtering is applied based on the solar zenith angle (see Section 3.1). Due to the yearly cycle of this geometry parameter, there are specific times of the year where there are no data available above specific latitudes (e.g., latitudes above 50-60 degrees in the Northern hemisphere winter).

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 every 15th orbit (once every 25 hours). 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 was 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, since the change from VCM to ECM, different.

4.4 Mission Operations Changes

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.

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

6.1.1 Version 02.03.01

New fields added

```
/PRODUCT/SUPPORT_DATA/DETAILED_RESULTS/maximum_reflectance_NIR  
/PRODUCT/SUPPORT_DATA/DETAILED_RESULTS/maximum_reflectance_SWIR
```

6.1.2 Version 02.02.00

New fields added

```
/METADATA/QA_STATISTICS attribute number_of_missing_scanlines  
/METADATA/QA_STATISTICS attribute  
number_of_max_num_outlier_exceeded_error_occurrences  
  
/METADATA/GRANULE_DESCRIPTION attribute CollectionIdentifier
```

Removed fields

```
/METADATA/ISO_METADATA/gmd:identificationInfo/gmd:spatialResolution
```

Renamed fields

```
/PRODUCT/qa_value attribute valid_min_  
→ /PRODUCT/qa_value attribute valid_min
```

```
/PRODUCT/qa_value attribute valid_max_  
→ /PRODUCT/qa_value attribute valid_max
```

```
/METADATA/QA_STATISTICS attribute number_of_aai_warning_occurrences  
→ /METADATA/QA_STATISTICS attribute number_of_AAI_warning_occurrences
```

6.1.3 Version 01.04.00

There are no format changes with respect to the previous version.

6.1.4 Version 01.03.00

New fields added

```
/PRODUCT/SUPPORT_DATA/INPUT_DATA/eastward_wind  
/PRODUCT/SUPPORT_DATA/INPUT_DATA/northward_wind
```

7 Product Availability

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

Information on data handling tools is available from the TROPOMI web page <http://www.tropomi.eu/tools>

For further questions regarding S5P/TROPOMI data products please contact 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:

https://sentinels.copernicus.eu/documents/247904/690755/Sentinel_Data_Legal_Notice

8 References

- [RD01] 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
url: <https://sentinels.copernicus.eu/documents/247904/2474724/Sentinel-5P-Calibration-and-Validation-Plan.pdf>
- [RD02] Algorithm Theoretical Baseline Document for Sentinel-5 Precursor Methane Retrieval,
source: SRON ref: SRON-S5P-LEV2-RP-001
url: <https://sentinels.copernicus.eu/documents/247904/2476257/Sentinel-5P-TROPOMI-ATBD-Methane-retrieval>
- [RD03] Sentinel-5 precursor/TROPOMI Level 2 Product User Manual Methane
source: KNMI; ref: SRON-S5P-LEV2-MA-001
url: <https://sentinels.copernicus.eu/documents/247904/2474726/Sentinel-5P-Level-2-Product-User-Manual-Methane>
- [RD04] Sha, M. K., Langerock, B., Blavier, J.-F. L., Blumenstock, T., Borsdorff, T., Buschmann, M., Dehn, A., De Mazière, M., Deutscher, N. M., Feist, D. G., García, O. E., Griffith, D. W. T., Grutter, M., Hannigan, J. W., Hase, F., Heikkinen, P., Hermans, C., Iraci, L. T., Jeseck, P., Jones, N., Kivi, R., Kumps, N., Landgraf, J., Lorente, A., Mahieu, E., Makarova, M. V., Mellqvist, J., Metzger, J.-M., Morino, I., Nagahama, T., Notholt, J., Ohyama, H., Ortega, I., Palm, M., Petri, C., Pollard, D. F., Rettinger, M., Robinson, J., Roche, S., Roehl, C. M., Röhling, A. N., Rousogenuous, C., Schneider, M., Shiomi, K., Smale, D., Stremme, W., Strong, K., Sussmann, R., Té, Y., Uchino, O., Velasco, V. A., Vigouroux, C., Vrekoussis, M., Wang, P., Warneke, T., Wizenberg, T., Wunch, D., Yamanouchi, S., Yang, Y., and Zhou, M.: Validation of methane and carbon monoxide from Sentinel-5 Precursor using TCCON and NDACC-IRWG stations, *Atmos. Meas. Tech.*, 14, 6249–6304, <https://doi.org/10.5194/amt-14-6249-2021>, 2021.
- [RD05] Algorithm theoretical basis document for the TROPOMI L01b data processor
source: KNMI; ref: S5P-KNMI-L01B-0009-SD; issue: 9.0.0; date: 2019-07-19;
url: <https://sentinels.copernicus.eu/documents/247904/2476257/Sentinel-5P-TROPOMI-Level-1B-ATBD>

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
CH ₄	Methane
ECM	Enterprise Cloud Mask
ESA	European Space Agency
ESL	Expert Support Laboratory
KNMI	Royal Netherlands Meteorological Institute / Koninklijk Nederlands Meteorologisch Instituut
MPC	Mission Performance Centre
NDACC	Network for the Detection of Atmospheric Composition Change
OFFL	Offline
PRF	Product Readme File
PUM	Product User Manual
ROCVR	Routine Operations Consolidated Validation Reports
RPRO	Reprocessing
SEOM-IAS	Scientific Exploitation of Operational Missions – Improved Atmospheric Spectroscopy Databases
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