



S5P Mission Performance Centre Carbon Monoxide [L2__CO____] Readme



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

1 Summary

This is the Product Readme File (PRF) for the Copernicus Sentinel 5 Precursor Tropospheric Monitoring Instrument (S5P/TROPOMI) Carbon Monoxide total column level 2 data product and is applicable for the Offline (OFFL) and Near Real Time (NRTI) timeliness data product.

A change in the Copernicus Sentinel 5P operations scenario increasing the 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_CO**_____

Example filename for the OFFL product:

S5P_OFFL_L2_CO_____20180702T205825_20180702T223955_03724_01_010002_20180708T202237.nc

Example filename for the NRTI product:

S5P_NRTI_L2_CO_____20180601T130316_20180601T130816_03280_01_010001_20180601T133329.nc

The file name convention is described in more detail in the Product User Manual (PUM) [RD03]. The OFFL product has the following Digital Object Identifier (DOI): <http://doi.org/10.5270/S5P-1hkp7rp>, for the NRTI product a corresponding identifier is not applicable.

This 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 `carbonmonoxide_total_column`, which gives the total atmospheric column between the surface and the top of atmosphere. The respective random error originating from the spectral fit is given in the `carbonmonoxide_total_column_precision`. As a user guideline for the data quality a `qa_value` is given with the data. 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.

The NRTI data stream delivers the CO column data product within 3 hours after sensing, whereas the OFFL data product is available a few days after acquisition. Because of the different timeliness, the NRTI product is given in 5 min data granules whereas the OFFL data product per satellite orbit. Both the OFFL and NRTI processing chains employ the same algorithm. Since processor version 01.03.02, the same configuration settings are used for both data streams and so the data products are expected to be of the same quality. For earlier versions, the NRTI and OFFL data product differ in the way the solar irradiance measurements are used. The NRTI processing requires the L1B reflectance spectra as input to the retrieval, whereas the OFFL processing is based on the Earthshine radiance measurements and uses a spectral deconvolution of the solar irradiance spectra during the algorithm initialization to infer a line-by-line solar spectrum as an input to the retrieval. More details on the two processing streams are given in the product Algorithm Theoretical Basis Document (ATBD) [RD02].

Independent validation by MPC Cal/Val experts and the Sentinel-5 Precursor Validation Team (S5PVT) concludes that the OFFL CO 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 MOPITT.

A bias of <10% found in the data comparisons is well within the mission requirements (Table 1) of $\leq 15\%$. The scatter of the data around this bias also complies with mission requirements of $\leq 10\%$. The comparison of S5p TROPOMI and MOPITT CO total columns supports the findings of the data product validation with ground-based measurements. The NRTI product is subject to an additional positive bias of 3-4 % but the data quality also stays within the mission requirements.

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

Parameter	Data product	Vertical Resolution	Bias	Random
Total column	Carbon monoxide (CO)	Total column	15%	10%

Table 1: Mission data requirements for the CO product, extracted from [RD01]

2 Processing baseline description

Table 2 contains the history of the CO processor versions. Note that the processor version for CO 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 CO product.

Processor Version	In operation from	In operation until	Relevant improvements
01.03.02	OFFL: orbit 8815, 201906-26 NRTI: orbit 8906, 2019-07-03	Current version	OFFL and NRTI processing chains employ the same algorithm since this version
01.03.01	OFFL: orbit 7907, 2019-04-23 NRTI: orbit 8000, 2019-04-30	Orbit 8814, 2019-06-26 Orbit 8906, 2019-07-03	No changes with respect to previous version
01.03.00	OFFL: orbit 7425, 2019-03-20 NRTI: orbit 7519, 2019-03-27	Orbit 7906, 2019-04-23 Orbit 7999, 2019-04-30	Added new variables: <code>eastward_wind</code> and <code>northward_wind</code>
01.02.02	RPRO: orbit 2818, 2018-04-30 OFFL: orbit 5833, 2018-11-28 NRTI: orbit 5932, 2018-12-05	Orbit 3847, 2018-07-11 Orbit 7424, 2019-03-20 Orbit 7518, 2019-03-27	Sun glint was wrongly considered in the <code>qa_value</code> calculation in previous versions
01.02.00	OFFL: orbit 5236, 2018-10-17 NRTI: orbit 5741, 2018-11-22	Orbit 5832, 2018-11-28 Orbit 5929, 2018-12-05	Adjusted <code>qa_value</code> in case of eclipse
01.01.00	OFFL: orbit 3848, 2018-07-11	Orbit 5235, 2018-10-17	Correction of a bug for <code>qa_value</code> and updated definition
01.00.02	OFFL: orbit 3661, 2018-06-28	Orbit 3847, 2018-07-11	Initial operational version

Table 2: History of CO processor versions. In orange, the data versions that are no longer available to the users on the Pre-operations hub.

3 Product Quality

3.1 Recommendations for data usage

Both for the OFFL and NRTI product, it is recommended to use TROPOMI CO data associated with a quality assurance value `qa_value` > 0.5. The `qa_value` is provided as part of the CO data product and the definition used in the current data release is summarized in Table 3.

<code>qa_value</code>	Condition	Remark
1.0	$\tau_{\text{aer}} < 0.5$ and $z_{\text{cld}} < 500$ m	clear-sky and clear-sky like observations
0.7	$\tau_{\text{aer}} \geq 0.5$ and $z_{\text{cld}} < 5000$ m	mid-levels cloud
0.4	($\tau_{\text{aer}} \geq 0.5$ and $z_{\text{cld}} \geq 5000$ m) or ($\tau_{\text{aer}} \leq 0.5$ and $z_{\text{cld}} \geq 500$ m)	high clouds, experimental data set
0.0	$\text{irow} \leq 1$ or $\text{SZA} \geq 80^\circ$ or defective product	corrupted or defective data

Table 3: `qa_value` parameter definition

Here, $\text{irow} \leq 1$ filters out the two most westward pixels because of unresolved calibration issues. For low sun with Solar Zenith Angles $\text{SZA} \geq 80^\circ$ the retrieval is most sensitive to radiometric and retrieval errors due to the long light path through the atmosphere. We recommend using only data with a `qa_value` = 1 in case the averaging kernel is not applied. Data with a `qa_value` = 0.7 are of similar quality provided the averaging kernel is used to account for the vertical retrieval sensitivity in the presence of mid-level clouds. Quality assurance values of `qa_value` = 0.4 represent experimental data to be used with caution.

For further details, data users are encouraged to read the Product User Manual (PUM, [RD03]) and Algorithm Theoretical Basis Document (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

Since processor version 01.03.02, the same configuration settings are used for the NRTI and OFFL data processing streams, therefore the data products are expected to be of the same quality. This will be verified during the next months and the validation results of this section will be updated accordingly.

3.2.1 Status of product validation

This section presents a summary of the key validation results obtained by the Validation Data Analysis Facility (VDAF) of the S5p Mission Performance Centre (MPC) and by the S5p Validation Team (S5PVT). It contains preliminary results reported at the S5p First Public Release Validation Workshop (ESA/ESRIN, June 25-26, 2018). Individual contributions to the workshop are available in <https://nikal.eventsair.com/QuickEventWebsitePortal/sentinel-5p-first-product-release-workshop/sentinel-5p>, while up-to-date validation results and consolidated validation reports are available through the MPC VDAF website at <http://mpc-vdaf.tropomi.eu>.

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. The conclusions summarized hereafter need to be confirmed by a larger amount of co-locations, and extended over a full year 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_CO_____ OFFL and NRTI carbon monoxide total column data are routinely compared to reference measurements of the TCCON and NDACC network.

3.2.2.2 Satellites

Initial S5P/TROPOMI L2_CO_____ carbon monoxide total column data of the OFFL data stream have also been compared to MOPITT CO data.

3.2.2.3 Model

Initial S5P/TROPOMI L2_CO_____ OFFL and NRTI carbon monoxide total column data have also been compared to CAMS-IFS CO total column after assimilating MOPITT and IASI CO observations.

3.2.3 Validation results

For a first data quality assessment, the TROPOMI CO OFFL data product was compared with the near-real-time data analysis of the ECMWF Integrated Forecasting System (IFS) assimilating IASI and MOPITT observations of CO (Inness et al., 2015, Atmospheric Chemistry and Physics, doi:10.5194/acp-15-5275-2015), which are provided by the Copernicus Atmosphere Monitoring Service (CAMS). For this purpose, Borsdorff et al. 2018 (Geophys. Res. Lett.; doi:10.1002/2018GL077045). Collocated the TROPOMI CO retrieval with the 6 hourly CAMS CO fields, interpolating the CAMS data to the time and location of the individual TROPOMI measurement. Subsequently, the integration of the CAMS profile using the column averaging kernel provides the corresponding column density, accounting for the vertical retrieval sensitivity of TROPOMI. Overall, the TROPOMI and CAMS CO fields agree well with small mean difference of +3.2 % between the TROPOMI and CAMS CO data with a standard deviation of 5.5 %. Both data sets are strongly correlated with a Pearson correlation coefficient of 0.97. Analyses for the period 14-22 September 2018 showed that the NRTI data product has an additional bias of 3.6 % at the Northern Hemisphere and 4.2 % at the Southern Hemisphere.

The quality of the TROPOMI CO data product is validated in more detail using independent on-ground reference observations both for clear-sky and cloudy TROPOMI measurements. To this end, two independent validation activities were performed. First, Borsdorff et al., 2018 (Atmos. Meas. Tech. Discuss. Doi:10.5194/amt-2018-132) performed a first validation with CO observations at nine ground-based FTS stations operated by the TCCON network. For the comparison, the authors used TROPOMI observations co-located with the TCCON sites by selecting all TROPOMI retrievals from the same day within a radius of 50 km around each station. The retrieved CO column of TROPOMI is adapted to the altitude of the validation ground site. With the limited data available at the time of their study, Borsdorff et al. found good agreement with a small mean bias of TROPOMI CO OFFL (NRTI) product versus TCCON of 6.0 ppb (8.9 ppb) for clear-sky, 6.2 ppb (6.3 ppb) for cloudy-sky TROPOMI retrievals and 5.8 ppb (8.0 ppb) for the combination of both with a station-to-station deviation of 3.9 ppb (4.2 ppb) for clear-sky, 2.4 ppb (4.8 ppb) for cloudy-sky, and 2.9 ppb (3.9 ppb) for the combination case. Furthermore, the mean standard deviation of the bias is 3.9 ppb (5.5 ppb) for clear-sky, 2.4 ppb (4.3 ppb) for cloud-sky, and 2.9 ppb (5.2 ppb) for the combination. The numbers in parentheses refer to the NRTI processing.

Additionally, S5p TROPOMI L2 carbon monoxide column data have been compared to correlative reference measurements acquired by FTIR instruments contributing to both the NDACC and TCCON networks using the S5p Validation Data Analysis Facility (VDAF) and TCCON4S5P AO project. The validated time period covers November 2017 to September 2018 for the OFFL product and May 2018 to September 2018 for the NRTI product. Using similar filter criteria, the S5p MPC Validation Data Analysis Facility (VDAF) study leads to the following preliminary conclusions:

- for all the reference stations, short scale temporal variations in the CO column as captured by ground-based instruments are reproduced very similarly by S5p OFFL. This overall good agreement is corroborated by Pearson correlation coefficients well above 0.7 and an average of 0.9 for OFFL and 0.85 for NRTI.

- the mean relative difference between S5p and reference data over the entire ground-based networks is of the order of +6% for OFFL and +10% for NRTI. The mean relative difference may exceed 10% at stations with few co-locations. This falls well within the mission requirements (bias at most 15%).
- The 1- σ spread of the relative differences (between S5p and reference data) around its mean value is on average for both NRTI and OFFL 4-5% and rarely exceeds 7%. Combining random errors in satellite and reference measurements with irreducible co-location mismatch effects, this value can be taken as a conservative upper limit of the random uncertainty on the S5p measurements, which satisfies the mission requirements (random uncertainty <10%).

Overall, the OFFL and NRTI product quality of this initial dataset appears to comply with the S5p mission requirements of Table 1. Current conclusions are nevertheless based on a limited initial dataset of measurements and including cloudy scenes. The current validation analysis needs to be extended over a full year of measurements, hence, a full cycle of key influence quantities, in order to enable detection of potential patterns, dependences, seasonal cycles and longer-term features like drifts.

For more details on the validation results against the NDACC and TCCON networks, the user is referred to the S5p MPC Validation Data Analysis Facility website at <http://mpc-vdaf.tropomi.eu>.

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 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 carbon monoxide product and also at preliminary validation results.

Stripes

Single TROPOMI overpasses show stripes of erroneous CO values < 5% in the flight direction, probably due to calibration issues of TROPOMI. Considering high-frequency variations of CO measurements across flight direction per orbit, stripe pattern can be inferred by median filtering of the detected features in flight direction and subsequently be removed from the data by the users. Boersma et al. (2011) suggested a similar approach to improve the quality of the NO₂ data product of the Ozone Monitoring Instrument. For corrections on the operational product, this aspect will be the subject of future investigations of the instrument calibration key data.

Metadata values exchanged

The global attributes `geospatial_lon_min` and `geospatial_lon_max` values are exchanged; therefore, the user is advised to switch the values for these fields, making note that the `geospatial_lat_min` and `geospatial_lat_max` values are correct. This is an issue traceable to L1b data (version 01.00.00) and is corrected in the following versions of the Level 1B processor.

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 6th August 2019. Note that, after this operations change, the metadata/Attributes fields 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 second half of 2020.

4.2 Solved Data Quality Issues

QA value (solved in version 01.02.02)

Sun glint is wrongly considered in the calculation of the `qa_value`. This is corrected since the activation of version 01.02.02 (December 2018, see Table 2).

Orbit numbering in NRTI and OFFL (solved in version 01.02.02)

Note that NRTI orbit numbers are set with respect to the downlink orbit while OFFL orbit numbers are set with respect to the equator crossing time. This creates an inconsistency between the NRTI and OFFL orbit numbers, which is removed with the activation of processor version 01.02.02 (December 2018, see Table 2).

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 (feature)

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.

5 Algorithm Change Record

For a detailed description of the L2__CO____ 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.

For OFFL data the product is stored as a single file per satellite orbit, for NRTI data the product is stored as multiple files per orbit.

Please note that consecutive data granules of the NRTI product show an overlap of about 12 scan lines.

Details of the data format are provided in the Product User Manual (PUM) [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

All S5P/TROPOMI data are available on the Copernicus Open Data 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.

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;
url: <https://sentinel.esa.int/documents/247904/2474724/Sentinel-5P-Calibration-and-Validation-Plan.pdf>
- [RD02] Algorithm Theoretical Baseline Document for Sentinel-5 Precursor: Carbon Monoxide Total Column Retrieval,
source: SRON **ref:** SRON-S5P-LEV2-RP-002,
url: <https://sentinel.esa.int/documents/247904/2476257/Sentinel-5P-TROPOMI-ATBD-Carbon-Monoxide-Total-Column-Retrieval>
- [RD03] Sentinel-5 precursor/TROPOMI Level 2 Product User Manual Carbon Monoxide
source: KNMI; **ref:** SRON-S5P-LEV2-MA-002;
url: <https://sentinel.esa.int/documents/247904/2474726/Sentinel-5P-Level-2-Product-User-Manual-Carbon-Monoxide>

More information on this data product is available from the 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
CO	Carbon Monoxide
DOI	Digital Object Identifier
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
NRTI	Near Real Time
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
VDAF	Validation Data Analysis Facility