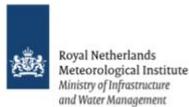




S5P Mission Performance Centre OFFL Tropospheric Ozone [L2__O3_TCL] Readme



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|-----------------|---|--|
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CHANGE LOG

| Reason for change | Issue | Revision | Date |
|--|-------|----------|------------|
| <ul style="list-style-type: none">Table 2: addition of version 01.01.08Section 4.2: addition of paragraph on version 01.01.08 | 1 | 4 | 19/03/2020 |
| Updates for processor version 02.01.03 | 2 | 0 | 16/07/2020 |
| Table 2: updates for processor version 02.01.04 | 2 | 1 | 11/12/2020 |
| Table 2: updates for processor version 02.02.01 | 2 | 2 | 05/07/2021 |
| <ul style="list-style-type: none">Table 2: updates for processor version 02.03.00Section 7: addition of link to major S5p mission data gaps | 2 | 3 | 11/03/2022 |
| Table 2: updates for processor version 02.04.01 | 2 | 4 | 27/07/2022 |
| Table 2: addition of reprocessed data, processor version 02.04.01 | 2 | 5 | 04/04/2023 |
| Table 2: updates for processor version 02.05.00 | 2 | 6 | 20/07/2023 |

1 Summary

This is the Product Readme File (PRF) for the Copernicus Sentinel 5 Precursor Tropospheric Monitoring Instrument (S5P/TROPOMI) Tropospheric Ozone Level 2 data product and is applicable for the Offline timeliness product (OFFL) and for the reprocessed (RPRO) dataset.

Product Identifier: **L2__O3_TCL**

Examples of filename:

S5P_OFFL_L2__O3_TCL_20190729T000957_20190803T130450_09312_01_020103_20200602T130019.nc
 S5P_RPRO_L2__O3_TCL_20220727T114816_20220802T123336_24844_03_020401_20230329T142508.nc

Please note that two metadata fields inside the RPRO products are slightly different with respect to the filename. For the example above:

- The product id inside the global attributes is:
`id = "S5P_OFFL_L2__O3_TCL_20220727T114816_20220802T123336_24844_01_020401_20230329T142900.nc"`
- The processing mode in the group attributes is:
`processingMode = "OFFL"`

This product has the following doi: <https://doi.org/10.5270/S5P-hcp112m>

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>.

An S5p L2__O3_TCL data file (one per day) contains two tropospheric ozone data sets, retrieved by different algorithms and they encompass different altitude ranges:

- `ozone_tropospheric_vertical_column` which provides the tropical tropospheric ozone column between the surface and a fixed pressure level of 270 hPa, based on the Convective Cloud Differential (CCD) algorithm.
- `ozone_upper_tropospheric_mixing_ratio` which provides the mean volume mixing ratio in the tropics over a variable height range (5 km minimum, 17 km maximum), it is retrieved using the Cloud Slicing Algorithm (CSA). **This product is not yet operational.**

In the following, the CSA product will not be discussed since the respective processor is not activated. **The CSA variables** are present in the data files, but all corresponding entries are **set to a fill value** for the time being.

The CCD data set is based on the offline S5p L2_O3___OFFL total ozone column data set and covers the tropical band between 20° South and 20° North. Each product contains a map of the 3-day running average of the clear-sky tropospheric ozone column on a fixed 0.5° (latitude) by 1° (longitude) grid. The associated `_precision` variable is based on the standard deviation of all tropospheric ozone columns within a bin. A quality assurance value (`qa_value`) is included and, to obtain the best data quality, it is currently recommended to only use pixels with a `qa_value > 0.7`.

Note: starting from processor version 2.4.1, new improved Level 1b version 2.1 [RD06] data products are used to process the OFFL Ozone data, which is the main input for the Tropospheric Ozone.

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

| Parameter | Data product | Vertical Resolution | Bias | Random |
|-----------|-------------------------|---------------------|------|--------|
| Ozone | Tropospheric ozone OFFL | tropospheric column | 25% | 25% |

Table 1: Tropospheric Ozone product uncertainty requirements

2 Processing baseline description

Table 2 contains a history of the O3-TCL processor versions. Note that the processor version for O3-TCL is changing when there is a change to any of the products belonging to the UPAS processor suite (O3 NRTI, O3 OFFL, O3-TCL, CLOUD, SO2, HCHO,) even if the change is not affecting the O3-TCL product.

Orbit numbers are not provided in Table 2 because each (daily) product represents the 3-day running average of the tropospheric ozone column, and thus the orbit number written in the filename is not meaningful (i.e., the product does not cover only that specific orbit).

| Processor Version | In operation from | In operation until | Relevant Improvements |
|-------------------|--------------------------------------|--------------------------|---|
| 2.05.00 | OFFL: 2023-07-04 | Current version | No changes with respect to previous version |
| 02.04.01 | OFFL: 2022-07-06 RPRO: 2018-04-30 | 2023-07-03 2022-08-03 | No changes in algorithm with respect to previous version. Note 1: It is recommended to use the RPRO products between 2022-07-06 – 2022-08-03, period for which also OFFL products are available. This, because the OFFL products in that range will be removed. Note 2: starting from this processor version 2.4.1, new improved Level 1b version 2.1 [RD06] data products are used to process the OFFL Ozone data, which is the main input for this product. |
| 02.03.00 | OFFL: 2022-02-23 | 2022-07-05 | No changes with respect to previous version |
| 02.02.01 | OFFL: 2021-07-15 | 2022-02-22 | Updates impacting the CLOUD input product: <ul style="list-style-type: none"> - New cloud-free maps based on 3 years of TROPOMI data - Improved handling of snow / ice conditions - Improved scan angle correction based on 3 years of TROPOMI - Optimized for the new L1b V2.0 input - New fallback surface albedo climatology based on 3 years of TROPOMI data - Improved clear-sky filtering in background correction Note: starting from this processor version 2.2.1, new improved Level 1b version 2.0 [RD06] data products are used to process the OFFL Ozone data, which is the main input for this product. |
| 02.01.04 | OFFL: 2020-11-18 | 2021-06-26 | Solved a problem that appeared when a certain combination of inputs was provided to the processor |
| 02.01.03 | OFFL: 2020-07-13 | 2020-11-17 | - New surface albedo retrieval algorithm (GE_LER) from TROPOMI for the NRTI O3 and CLOUD product replaces the climatologies (affects CLOUD input product) |

| | | | |
|----------|--------------------------------------|--------------------------|--|
| | | | <ul style="list-style-type: none"> - New OCRA cloud-free maps based on TROPOMI instead of OMI (affects CLOUD input product) - New cloud flags have been introduced (e.g. ice-clouds) - The required interpolation of cloud properties co-registration between band 3-4 and band 6 due to the instrument co-registration issue has been improved in the CLOUD product - Updated metadata generation to reflect the improved spatial resolution after 6th Aug 2019 - Improved handling of the ECMWF information, reading and deriving snow-ice information and propagating wind-information in the level 2 products - Fixed inconsistency in the surface / effective scene pressure calculation in the O3 OFFL algorithm - Improved the <code>qa_value</code> determination - Improved the prior value of the effective scene albedo (affects O3 OFF input data) - Fixed inconsistency in the surface/effective scene pressure calculation in the algorithm - Invalid values of <code>geolocation_flags</code> set to correct values - New variables added (see section 6.1) |
| 01.01.08 | OFFL: 2020-02-26 | 2020-07-12 | Version correcting a problem in the filename. This problem prevented the availability of OFFL data between 11/09/2019 - 16/10/2019. Reprocessed data covering this period will be made available in the future |
| 01.01.07 | OFFL: 2019-04-16 | 2020-02-25 | Correction of the CLOUD product handling when cloud fractions were less than 5%. This caused evident gaps in Ozone OFFL input data with version 01.01.06 (see section 4.2) |
| 01.01.06 | OFFL: 2019-03-21 | 2019-04-15 | <ul style="list-style-type: none"> - Correction of occasional, too high cloud top pressure (Cloud as Reflecting Boundaries, CRB) in the tropics that caused the OFFL total ozone columns to be biased low (Ozone OFFL is an input to Tropospheric Ozone) (see section 4.2) - Updated surface classification climatology (for input Ozone OFFL) - Fixed a bug in the interpolation of the surface albedo climatology (for input Ozone OFFL) |
| 01.01.05 | OFFL: 2018-12-14 OFFL: 2018-04-30 | 2019-03-20 2018-12-12 | Initial operational version. These are reprocessed data. |

Table 2: History of Tropospheric Ozone processor versions.

3 Product Quality

3.1 Recommendations for data usage

In order to obtain the best data quality, it is currently recommended to only use TROPOMI tropospheric column grid cells with a `qa_value` strictly larger than 0.7. Lower thresholds will degrade the data quality with the appearance of biases between latitude bands (see Section 4).

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

3.2 Validation results

Independent validation by the S5p MPC Cal/Val experts and the S5PVT conclude that the OFFL tropospheric ozone data is in good overall agreement (i) with reference measurements collected by ozonesondes, and (ii) with corresponding satellite data products from OMI and GOME-2.

TROPOMI tropospheric ozone column data are biased high with respect to coincident ozonesonde data, on average by 2.8 DU. A small negative bias of 0.1 DU is found in TROPOMI data compared to the OMI data and an overestimation of 2.3 DU compared to GOME-2. These bias estimates are within the mission requirements of maximum 25% (~5 DU). The dispersion of the comparison data around this bias ranges between 2.6 and 4.6 DU, which complies with mission requirements of 25% as well. Further studies that consider random uncertainty from co-location mismatch, indicate that TROPOMI single-measurement random uncertainty is 1.5-2.5 DU (~8-13%).

More detailed (e.g. dependences on influence quantities) and up to date validation results are available in the ROCVR reports that are accessible through the MPC VDAF website at <http://mpc-vdaf.tropomi.eu>. The reports are issued quarterly.

4 Data Quality Remarks

The following data quality issues are currently known for L2_O3_TCL OFFL, when applying the recommended `qa_value > 0.7` screening. These issues should be kept in mind when analysing the tropospheric ozone product and when interpreting the preliminary validation results.

4.1 Known Data Quality

Optimization on-going

Some settings within the algorithm (e.g. `cloud_height_minimum`) are still object of further optimisation, therefore the respective values can differ between the ATBD [RD02] and the data files. In this case, it is recommended to use the values in the files as they are directly written by the retrieval algorithm.

Latitudinal stripping

A latitudinal striping structure (<~1-2 DU) occurs in some of the products. This is caused by the basic assumption that the stratospheric reference column is constant for each 0.5° latitude band. An update of the smoothing algorithm for the stratospheric reference reduced the problem. This striping occurs especially at the northern and southern edges of the tropical band, it is recommended to check the `qa_value` in this case. Relaxing the `qa_value` threshold to values below 0.7 increases the frequency and magnitude of the stripes, so this should only be done with great care.

TROPOMI Orbit structures

For some files, structures of up to 5 DU following the TROPOMI-orbit can be seen in the tropospheric ozone column distribution. These are probably caused by an under-sampling, and cannot be solved easily. If possible, the user might reduce the temporal resolution by averaging the tropospheric ozone column over several days.

4.2 Solved Data Quality

Outliers in CLOUD product (solved in version 01.01.06)

The tropospheric ozone data are based on the OFFL ozone total column level 2 data. Therefore, quality issues of the total column and cloud datasets [RD04, RD05] affect the tropospheric ozone data. The OFFL product makes use of the Cloud as Reflecting Boundaries (CRB) parameters from the CLOUD operational product. Some occasional outliers have been identified in the CRB cloud top pressure fields (CTP too high) in Tropical regions. For such events, the OFFL total ozone columns are biased low. A correction in the cloud algorithm has been developed and was implemented in version 01.01.06 (see Table 2).

Data gaps in input Ozone OFFL product in version of 01.01.06 (solved in version 01.01.07)

OFFL Ozone data processed with version 01.01.06 show evident gaps due to an inconsistency in the input cloud parameters: when the cloud fraction is very low (between 0 and 5%) the correlated cloud parameters (cloud top height, etc) are set to fill values (invalid). But because the cloud fraction was not 0%, the Ozone algorithm assumed that the cloud parameters were valid causing problems during the retrieval and leading to gaps in the final OFFL Ozone products. This inconsistency has been corrected with version 01.01.07 of the processor (see Table 2) where original cloud fractions < 5% are set to 0% during the cloud processing. Note that the original cloud-fraction is still saved in the `cloud_fraction_a_priori` variable of the CLOUD product.

Data gap between 11/09/2019 - 16/10/2019 (solved in version 01.01.08)

A problem in the filename configuration prevented the availability of data between 11/09/2019 - 16/10/2019. The problem was solved with version 01.01.08. A workaround solution was put in place on 16 October 2019 allowing the correct generation of filenames and the subsequent availability of data still with version 01.01.07.

4.3 Mission Operations Change

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. This change affects the resolution of the Ozone OFFL total column which is an input to the Tropospheric Ozone product. The resolution of the Tropospheric Ozone product remains unchanged and fixed to a 0.5° (latitude) by 1° (longitude) grid.

5 Algorithm Change Record

For a detailed description of the L2__O3_TCL algorithms, please refer to the ATBD [RD02]. Due to non-optimized settings the `ozone_upper_tropospheric_mixing_ratio` **entries and all related CSA variables are set to a fill value in versions 01.01.05 and later ones.**

6 Data Format

The product is stored as a NetCDF4 file. The NetCDF4 file contains both the data and the metadata for the product. Usually, one data file is produced per day.

Details of the data format are provided in the Product User Manual (PUM) [RD03].

6.1 Data format changes

6.1.1 Version 02.04.01

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

6.1.2 Version 02.03.00

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

6.1.3 Version 02.02.01

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

6.1.4 Version 02.01.04

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

6.1.5 Version 02.01.03

New fields added

/PRODUCT/SUPPORT_DATA/DETAILED_RESULTS/surface_pressure

7 Product Availability

The S5p Ozone Tropospheric OFFL data are available from the Copernicus Open Access Hub <https://scihub.copernicus.eu>.

The list of major mission data gaps due to acquisition faults or satellite/instrument disruption is available at <https://sentinel.esa.int/web/sentinel/missions/sentinel-5p/mission-status>. For those periods the data are permanently lost.

Information on data handling tools is available from the 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 Operation Phase
source: ESA; **ref:** ESA-EOPG-CSCOP-PL-0073
url: <https://sentinels.copernicus.eu/documents/247904/2474724/Sentinel-5P-Calibration-and-Validation-Plan.pdf>
- [RD02] Sentinel-5 precursor/TROPOMI Level 2 Algorithm Theoretical Basis Document O3 Tropospheric Column
source: DLR; **ref:** S5P-L2-IUP-ATBD-400C
url: <https://sentinel.esa.int/documents/247904/2476257/Sentinel-5P-ATBD-TROPOMI-Tropospheric-Ozone>
- [RD03] Sentinel-5 precursor/TROPOMI Level 2 Product User Manual O3 Tropospheric Column
source: DLR; **ref:** S5P-L2-DLR-PUM-400C
url: <https://sentinel.esa.int/documents/247904/2474726/Sentinel-5P-Level-2-Product-User-Manual-Ozone-Tropospheric-Column>
- [RD04] S5P Mission Performance Centre OFFL Total Ozone [L2__O3____] Readme
Source: DLR, BIRA, ESA **ref:** S5P-MPC-BIRA-PRF-O3-OFFL
url: <https://sentinel.esa.int/documents/247904/1848259/S5P-Readme-OFFL-Total-Ozone.pdf>
- [RD05] S5P Mission Performance Centre Cloud [L2__cloud_] Readme
Source: DLR, BIRA, ESA **ref:** S5P-MPC-DLR-PRF-cloud
url: <https://sentinel.esa.int/documents/247904/3541451/Sentinel-5P-Cloud-Level-2-Product-Readme-File>
- [RD06] Algorithm theoretical basis document for the TROPOMI L01b data processor
source: KNMI; **ref:** S5P-KNMI-L01B-0009-SD;
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 | Koninklijk Belgisch Instituut voor Ruimte-Aeronomie - Institut royal d'Aéronomie Spatiale de Belgique - Royal Belgian Institute for Space Aeronomy |
| CCD | Convective-Cloud Differential |
| CCI | ESA's Climate Change Initiative |
| CRB | Cloud as Reflecting Boundary |
| CSA | Cloud Slicing Algorithm |
| DLR | Deutsches Zentrum für Luft- und Raumfahrt – German Aerospace Centre |
| DU | Dobson Unit |
| ESA | European Space Agency |
| ESL | Expert Support Laboratory |
| GOME-2 | Global Ozone Monitoring Experiment-2 |
| KNMI | Koninklijk Nederlands Meteorologisch Instituut – Royal Dutch Meteorological Institute |
| MPC | Mission Performance Centre |
| OFFL | Offline |
| OMI | Ozone Monitoring Instrument |
| PRF | Product Readme File |
| PUM | Product User Manual |
| ROCVR | Routine Operations Consolidated Validation Report |
| S5P | Sentinel-5 Precursor |
| S5PVT | Sentinel-5 Precursor Validation Team |
| SHADOZ | Southern Hemisphere ADditional OZonesonde programme |
| TROPOMI | TROPOspheric Monitoring Instrument |
| UPAS | Universal Processor for UV / VIS Atmospheric Spectrometers |
| VDAF | Validation Data Analysis Facility |