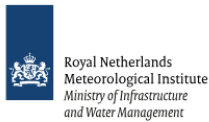




# S5P Mission Performance Centre OFFL Tropospheric Ozone [L2\_\_O3\_TCL] Readme



document number	S5P-MPC-DLR-PRF-O3-TCL	
issue	2.0	
date	2020-07-16	
product version	V02.01.03	
status	Released	
Prepared by	K.-P. Heue (DLR) F. Romahn (DLR) D. Hubert (BIRA-IASB) J.-C. Lambert (BIRA-IASB)	MPC Product Lead MPC Processor Lead MPC Validation Coordinator MPC ESL-VAL Lead
Reviewed by	D. Loyola (DLR) J. P. Veefkind (KNMI),	MPC ESL-L2 Lead MPC Technical Manager
Approved by	A. Dehn (ESA) C. Zehner (ESA)	ESA Data Quality Manager ESA Mission Manager

MPC Contributors	J. Granville (BIRA-IASB) K.-U. Eichmann (Uni Bremen) D. Loyola (DLR) P. Valks (DLR) J. Xu (DLR) L. Saavedra de Miguel (ESA/Serco)	MPC ESL-VAL Contributor MPC ESL-L2 Product Contributor MPC ESL-L2 Lead MPC ESL-L2 Product Contributor MPC ESL-L2 Product Contributor ESA S5p Mission Support
S5PVT Contributors	A. Keppens (BIRA-IASB)	S5PVT PI, CHEOPS-5P Project
Signatures	MPC Product Lead / PRF Editor	
	A. Dehn (ESA) – Data Quality Manager	
	C. Zehner (ESA) – Mission Manager	

## CHANGE LOG

Reason for change	Issue	Revision	Date
<ul style="list-style-type: none"><li>Table 2: addition of version 01.01.08</li><li>Section 4.2: addition of paragraph on version 01.01.08</li></ul>	1	4	19/03/2020
Updates for processor version 02.01.03	2	0	16/07/2020

# 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).

Product Identifier: **L2\_O3\_TCL**

Example filename:

S5P\_OFFL\_L2\_O3\_TCL\_20190729T000957\_20190803T130450\_09312\_01\_020103\_20200602T130019.nc

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 in order to obtain the best data quality it is currently recommended to only use pixels with a `qa_value > 0.7`.

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

The quality of the processor version 2.x.x has been assessed on a dedicated Test Data Set.

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
02.01.03	2020-07-13	Current version	<ul style="list-style-type: none"> <li>- New surface albedo retrieval algorithm (GE_LER) from TROPOMI for the NRTI O3 and CLOUD product replaces the climatologies (affects CLOUD input product)</li> <li>- New OCRA cloud-free maps based on TROPOMI instead of OMI (affects CLOUD input product)</li> <li>- New cloud flags have been introduced (e.g. ice-clouds)</li> <li>- 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</li> <li>- Updated metadata generation to reflect the improved spatial resolution after 6<sup>th</sup> Aug 2019</li> <li>- Improved handling of the ECMWF information, reading and deriving snow-ice information and propagating wind-information in the level 2 products</li> <li>- Fixed inconsistency in the surface / effective scene pressure calculation in the O3 OFFL algorithm</li> <li>- Improved the qa_value determination</li> <li>- Improved the prior value of the effective scene albedo (affects O3 OFF input data)</li> <li>- Fixed inconsistency in the surface/effective scene pressure calculation in the algorithm</li> <li>- Invalid values of geolocation_flags set to correct values</li> <li>- New variables added (see section 6.1)</li> </ul>
01.01.08	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	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	2019-03-21	2019-04-15	<ul style="list-style-type: none"> <li>- 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)</li> <li>- Updated surface classification climatology (for input Ozone OFFL)</li> <li>- Fixed a bug in the interpolation of the surface albedo climatology (for input Ozone OFFL)</li> </ul>
01.01.05	2018-12-14 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 version 1.x.x of 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 (V1.x.x) 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>. They are issued quarterly, and reports released after July 2020 include validation results based on processor version 2.x.x.

## 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 ( $\sim 1-2$  DU) occurs in some of the products. This is caused by the basic assumption that the stratospheric reference column is constant for each  $0.5^\circ$  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 New Variables (introduced with version 02.01.03)

/PRODUCT/SUPPORT\_DATA/DETAILED\_RESULTS/surface\_pressure

## 7 Product Availability

The S5p OFFL data are available from the Copernicus 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:

[https://sentinels.copernicus.eu/documents/247904/690755/Sentinel\\_Data\\_Legal\\_Notice](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>

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