S5P Mission Performance Centre
OFFL Tropospheric Ozone [L2__O3_TCL] Readme

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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).

A change in the Copernicus Sentinel 5P operations scenario, increasing the spatial resolution from 7.2 km to 5.6 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.

Product Identifier: **L2__O3_TCL**

Example filename:
S5P_OFFL_L2__O3_TCL_20180315T114925_20180321T123546_02172_01_010105_20181212T103132.nc

This product has the following doi: **10.5270/S5P-8aqg6um**.

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 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 fully operational**.

In the following, the CSA product will not be discussed until the respective processor has been finalized. **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 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.

Data product requirements from the S5p Calibration and Validation Plan [RD01] are in Table 1.

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

Table 1: Tropospheric Ozone product uncertainty requirements

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 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 3.1 DU or 16%. A small negative bias of less than ~1 DU is found in the data compared to the OMI data and an overestimation of less than 2 DU compared to GOME-2. Current bias estimates are within the mission requirements of maximum 25%. The scatter of the data around this bias is broadly compliant with mission requirements of 25%, but studies are ongoing to consolidate estimates of random uncertainty.

2 Processing baseline description

The following table 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 (SO2, HCHO, O3 NRTI, O3 OFFL, O3-TCL, CLOUD) even if the change is not affecting the O3-TCL product.

Processor Version	In operation from	In operation until	
01.01.05	Orbit 6059, 2018-12-14	Orbit 7421, 2019-03-20	Initial operational version
01.01.06	Orbit 7435, 2019-03-21	Orbit 7791, 2019-04-15	- 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)
01.01.07	Orbit 7804, 2019-04-16	Current version	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)

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

3.2.1 Status of product validation

This section presents a summary of the key validation results obtained by the S5p MPC Validation Data Analysis Facility (VDAF) and by the S5PVT. It contains results reported at the S5p Third Product Release meeting (February 20, 2019). Individual contributions to the meeting are archived at https://sentinel.esa.int/web/sentinel/technical-guides/sentinel-5p/calibration-validation-activities/sentinel-5p-third-products-release-workshop, 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 analysis, and on the period covered by the initial S5p dataset (November 2017 to January 2019). The conclusions summarized hereafter need to be confirmed by a larger amount of co-locations, and extended over a longer time series, in order to enable detection and quantification of potential patterns, dependences, seasonal cycles and longer-term features.

3.2.2 Validation approach

Routine validation of the S5P/TROPOMI L2__O3_TCL tropospheric ozone data products entails both qualitative, visual inspections of daily maps of product variables, and quantitative comparisons of these to independent measurements.

3.2.2.1 Ozonesonde network

Reference measurements by ozonesondes launched at nine sites in the ground-based SHADOZ network are compared to TROPOMI data in an operational fashion. The ozonesonde profile data are first quality controlled and then integrated over the vertical range of the S5p CCD product to obtain a comparable tropospheric column. Comparison statistics are computed from time series of coincident measurements at each station. The considerable difference in spatio-temporal sampling of S5p and the sonde network is taken into account qualitatively when interpreting the validation results.

3.2.2.2 Satellites

S5P/TROPOMI L2__O3_TCL tropospheric ozone column data are also compared to AURA/OMI and METOP-B/GOME-2 tropospheric ozone column data (GODFIT_v4 CCI). The algorithm was developed within ESA's Climate Change Initiative (CCI) based on the GODFIT total column data but the sampling was adapted to allow a more direct comparison to TROPOMI, i.e. 5 days averaging windows instead of monthly data and tropospheric top pressure set to 270 hPa instead of 200 hPa. The horizontal resolution of the OMI and GOME-2B data product was changed from 1.25°x2.5° to 1°x2°.

3.2.3 Validation results

Overall, the quality of the initial L2__O3_TCL OFFL v01.01.05 data products complies with the mission requirements: bias of max. 25% and random uncertainty of max. 15-25%.

Ground-based validation analyses carried out by an independent team (BIRA-IASB), and satellite intercomparisons carried out at DLR lead to the following preliminary conclusions:

- Geophysical structures such as the zonal wave-one pattern and the seasonal cycle are clearly visible in the tropospheric ozone column fields and these generally agree with expectations.
- However, artificial patterns due to sampling have been seen as well. There are sometimes artificial changes of <1-2 DU between neighbouring latitude bands and, occasionally, part of the temporal structure follows the progression of the S5p orbit. These artefacts become more pronounced when lowering the `qa_value` screening threshold to less than 0.7.
- When applying the recommended screening threshold, comparisons to ozonesonde show a positive bias in S5p measurements at all but one station (Figure 3.1). When averaged over the nine sites the S5p bias is +3.1 DU or +16%. The correlation between sonde and S5p data averages to 63%. The spread in the comparison time series ranges between 2-7 DU or 10-38%. More detailed studies are ongoing to quantify all sources of random uncertainty.
- Compared to the OMI tropospheric ozone column a small negative bias of less than 1 DU is found for S5p (Figure 3.2). For GOME-2B, the difference gets larger +1.8 DU. However, in this case, the difference in the overpass time and the respective atmospheric change has to be taken into account.

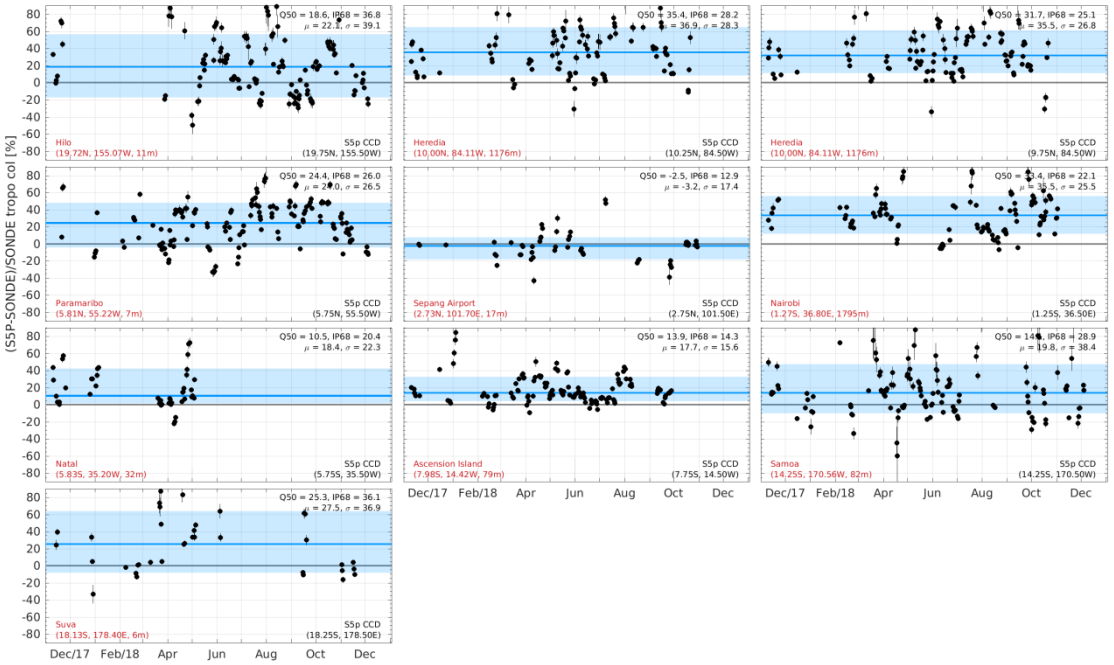

Figure 3.1: Relative difference time series of coincident S5p and ozonesonde tropospheric ozone column data, at nine SHADOZ sites (Heredia is located on the edge between two S5p grid cells). The blue line and shaded area represent the median and 68% percentile.

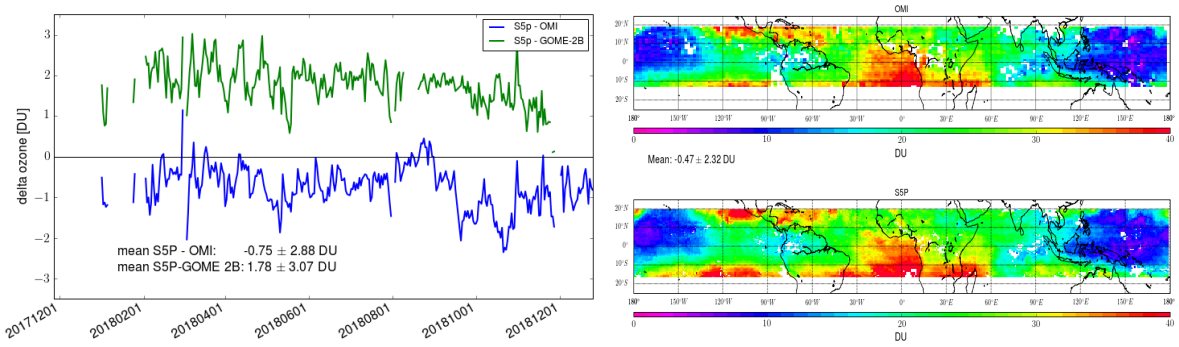

Figure 3.2: Comparisons to the CCI OMI and GOME_2B data product. Left: time series of the mean difference, right example comparison for 24th-29th July 2018.

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) can occur in some of the datasets. 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.

TROPOMI Orbit structures

For some files, structures following the TROPOMI-orbit can be seen in the tropospheric ozone column distribution. This is 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 at activation 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.

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 following 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

This document describes the first public release of the data product, therefore there are no changes to report.

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.

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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
S5P	Sentinel-5 Precursor
S5PVT	Sentinel-5 Precursor Validation Team
SCIAMACHY	SCanning Imaging Absorption spectroMeter for Atmospheric CHartographY
SHADOZ	Southern Hemisphere ADditional OZonesonde programme
TROPOMI	TROPOspheric Monitoring Instrument
VDAF	Validation Data Analysis Facility