S5P Mission Performance Centre
Readme OFFL Total Ozone

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1 Summary

This is the Product Readme File (PRF) for the public release of the Copernicus Sentinel 5 Precursor Tropospheric Monitoring Instrument (S5p/TROPOMI) Total Ozone Level 2 data product and is applicable for the Offline (OFFL) timeliness product.

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.

Product Identifier: **L2__O3____**

Example filename:

S5P_OFFL_L2__O3_____20180809T121633_20180809T135802_04258_01_010106_20180815T141816.nc

This product has the following Digital Object Identifier (DOI): https://doi.org/10.5270/S5P-fqouvyz

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 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 `ozone_total_vertical_column` which gives the total atmospheric column between the surface and the top of atmosphere. The respective random uncertainty originating from the spectral fit is given in the `ozone_total_vertical_column_precision field.`

Data product requirement from the S5p Calibration and Validation Plan [RD01]:

Parameter	Data product	Vertical Resolution	Bias	Random
Ozone	Total ozone OFFL	Total column	3.5-5%	1.6-2.5%

Table 1: Ozone Offline data products uncertainty requirements

Independent validation by Mission Performance Centre (MPC) Cal/Val experts and the Sentinel-5 Precursor Validation Team (S5PVT) conclude that version 01.01.06 of the OFFL ozone data is in good overall agreement with (i) reference measurements collected from global ground-based networks, and (ii) the corresponding satellite data product from Ozone Mapper and Profiling Suite (OMPS). The global bias with respect to the ground-based measurements is found to be below 1%, which is well within the mission requirements of maximum 3-4%. The biases at individual stations also satisfy this requirement. The scatter of the differences around this bias also complies with mission requirements of ±2.5%.

2 Processing baseline description

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

Please note that the processor version annotation in the filenames of orbits **4147** to **4158** are not correct. Those products are actually processed with the UPAS version 01.01.02, but in the filename it is written 01.01.01.

Processor Version	In operation from	In operation until	Relevant Improvements
01.01.02	OFFL: orbit 4147, 2018-08-01	Orbit 5832, 2018-11-28	Initial operational version
01.01.05	OFFL: orbit 5833, 2018-11-28	Orbit 7541, 2019-03-28	Inconsistency between pressure grid and averaging kernel values has been resolved (see section 4.2)
01.01.06	OFFL: orbit 7542, 2019-03-28	Orbit 7906, 2019-04-23	- Correction of occasional Cloud as Reflecting Boundaries (CRB) cloud top pressure field too high in Tropical regions that caused the OFFL total ozone columns to be biased low (see section 4.2) - Unit of `smoothing_error` parameter is mol.cm^{-2}, consistently with the other variables since this version. In previous versions it was provided in Dobson Units (see section 4.2) - Surface classification climatology updated - Fixed a bug in the interpolation of the surface albedo climatology
01.01.07	OFFL: orbit 7907, 2019-04-23	Current version	Correction of the CLOUD product handling when cloud fractions were less than 5%. This caused evident gaps in data with version 01.01.06 (see section 4.2)

Table 2: History of Ozone OFFL processor versions

3 Product Quality

3.1 Recommendations for data usage

The `qa_value` as currently provided in the L2 files is often too conservative and leads to a too stringent filtering if used. It is recommended **not** to use this variable to filter data but rather to use the criteria defined in section 4 for this.

For further details, data users are encouraged to read the Product User Manual (PUM) and Algorithm Theoretical Basis Document (ATBD) associated with this data product, both available on 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 Validation Data Analysis Facility (VDAF) of the S5p MPC and by the S5PVT. It contains preliminary results reported during the S5p Second Public Products Release Webex Meeting (September 28, 2018). Individual contributions to the workshop are archived in https://sentinel.esa.int/web/sentinel/technical-guides/sentinel-5p/calibration-validation-activities/sentinel-5p-second-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 first analysis, and on the period covered by the initial S5p dataset. The conclusions summarized hereafter, although very likely representative of the product quality, will need to be confirmed by a larger amount of co-locations, and extended over more than 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__O3____ total ozone column data are routinely compared to reference measurements acquired by instruments contributing to WMO's Global Atmosphere Watch: (1) Brewer and (2) Dobson UV spectrophotometers, and (3) NDACC zenith-sky DOAS UV-Visible spectrometers of the SAOZ type. Over the period tested, with respect to the reference data available at the time of this analysis, of the order of 20 to 200 co-locations have been identified at about 40 Brewer and Dobson sites and at 8 SAOZ sites, sampling many latitudes from the Arctic to the Antarctic.

3.2.2.2 Satellites

S5p/TROPOMI L2__O3____ OFFL total ozone columns are also compared to S5p/TROPOMI NRTI total ozone columns and to GODFIT and DOAS-type retrievals of total ozone from OMI/Aura, OMPS/Suomi-NPP, and GOME-2/MetOp-A,B, as well as OMPS/Suomi-NPP total ozone from NASA.

3.2.3 Validation results

Overall, the quality of the initial L2__O3____ OFFL v01.01.02 data product appears to comply with the mission requirements: a bias of max. 3.5-5% and a random uncertainty of max. ±2.5%.

Ground-based data comparisons carried out by an independent team (AUTH, BIRA-IASB, ECCC and LATMOS-CNRS), and satellite-based comparisons carried out at AUTH, BIRA-IASB, and DLR lead to the following preliminary conclusions:

- **Bias:** the systematic difference between S5p and reference ground-based data at individual stations rarely exceeds 2%, as depicted in Figure 1. The median bias calculated over the entire ground-based networks is of the order of 0-0.5%. Between 50˚S and 50˚N, the mean agreement with other satellite data is within 1% as well (Figure 2). This median bias value falls well within the mission requirements (max. bias of 3.5-5%).

- **Random difference:** the ±1σ spread of the differences (between S5p and reference data) around the median value rarely exceeds 2-3% for the comparisons with direct-sun instruments. Combining random errors in satellite and reference measurements with irreducible co-location mismatch effects, it is likely that the random uncertainty on the S5p measurements falls within mission the requirements of max. ±2.5%.
- **Dependence on influence quantities:** The analysis of potential dependence of the S5p bias and comparison spread on the Solar Zenith Angle (SZA), Air Mass Factor (AMF) and cloud fraction (CF) of the S5p measurement does not reveal yet any variation of the bias larger than 2% over the range of those influence quantities. Biases of -3% and +3% could exist at very small (<210K) and large (>240K) effective temperatures respectively, but this needs confirmation with more co-locations in these regimes. No bias larger than 1% is observed at more moderate effective temperatures. Note that differences w.r.t. DOAS-type satellite data products can increase up to a few percent at large SZA due to a more accurate retrieval algorithm in the OFFL processor.
- **Geographical patterns:** Maps of the bias between S5p and other satellite data sets reveal patterns correlating with weather patterns and atmospheric circulation features. These patterns are likely to be associated with differences in the modeling of the cloud properties, and also to differences in overpass times (e.g. 3.5 hours difference between S5p and GOME-2). The retrieval of the surface albedo in the OFFL product leads to reduced regional biases in comparison to satellite products still based on coarse and uncertain surface albedo climatologies (e.g. the S5p/TROPOMI NRTI product).
- **Short-term variability:** Qualitatively, at all of the 50 reference stations, short scale temporal variations in the ozone column as captured by ground-based instruments are reproduced very similarly by S5p. The overall good agreement is corroborated by Pearson correlation coefficients always above 0.95.

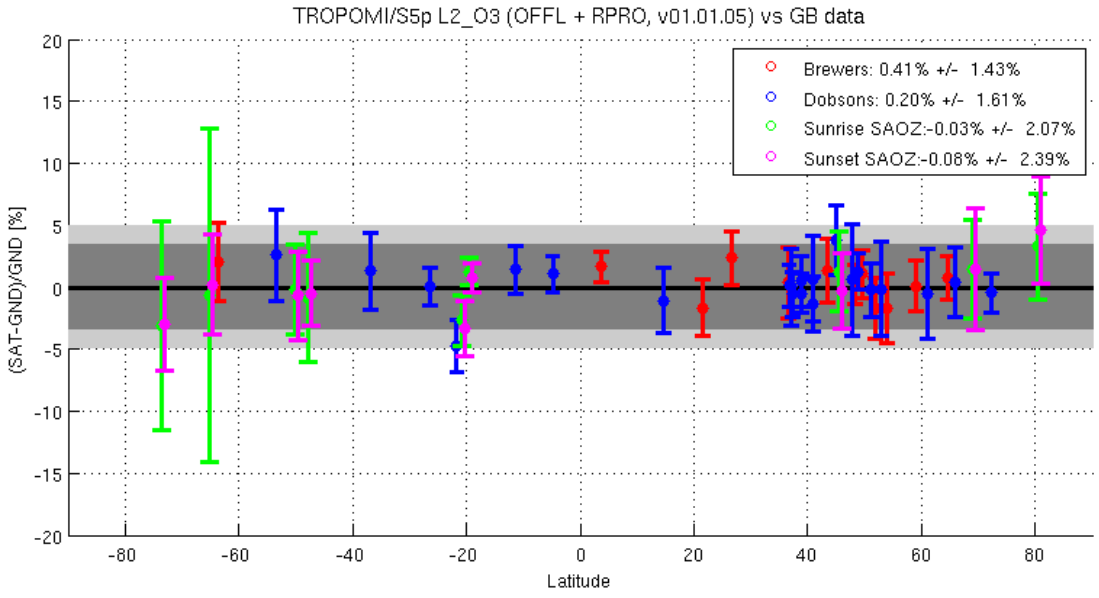

Figure 1 - Meridian dependence of the median and spread (±1 sigma) of the bias between S5p TROPOMI L2_O3 (PDGS OFFL processor v01.01.05, including reprocessed data) and ground-based (GB) reference ozone column data, represented at individual stations from the Antarctic to the Arctic and per reference measurement type (Brewer, Dobson and SAOZ). The values in the legend correspond to the median and spread of all median (per station) differences. For clarity, sunrise and sunset SAOZ results have been offset by -0.5˚ and +0.5˚ in latitude. The light and dark grey bands represent the mission requirements on systematic and random uncertainty respectively.

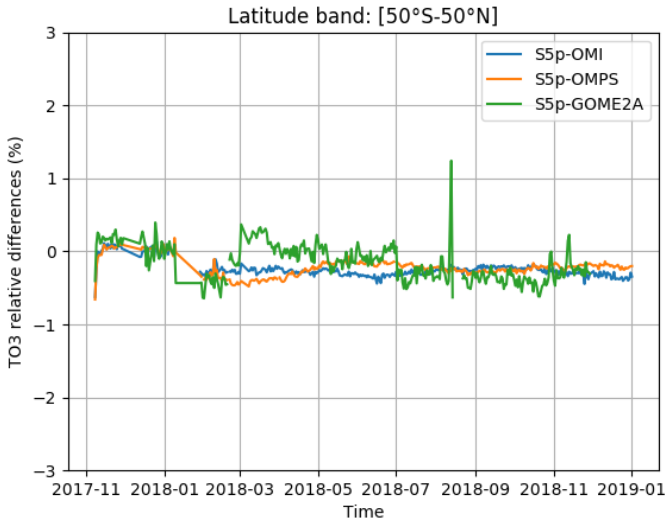

Figure 2 - Zonal mean relative differences between the total ozone S5p OFFL product and other satellite data sets generated with the same algorithm GODFITv4. Those differences averaged in the latitude band +/-50° are plotted as a function of time.

4 Data Quality Remarks

4.1 Known Data Quality

Currently, the following data quality issues are known, not covered by the quality flags, and should be kept in mind when looking at the total ozone product itself and also at preliminary validation results.

Related to the `qa_value`, the current approach to compute it results in to too low values at large solar zenith angles (>75˚), leading to a rejection of valid measurements at high latitudes if used to filter the product. Alternative approaches to compute `qa_value` are under investigation and are planned to be implemented in the future. Alternatively, the users can apply their own filters. For example, pixels with retrieved variables out of the following ranges should be used with care or rejected:

- `ozone_total_vertical_column` out of [0 to 0.45]
- `ozone_effective_temperature` out of [180 to 260]
- `ring_scale_factor` out of [0 to 0.15]
- `effective_albedo` out of [-0.5 to 1.5]

Bands 3-4 and 6 spatial misalignment

The band 3-4 (450 pixels per scanline) footprints are not fully aligned with the band 6 (448 pixels per scanline) footprints. In the worst case, the misalignment can be of the order of half a ground pixel. The OCRA algorithm retrieves the CF at Bands 3 and 4. This is an *a priori* to the ROCINN algorithm which works in band 6. Over heterogeneous scenes this miss-registration might have a large impact on the data quality. In the current products, a shift of two detector pixels between band 3-4 and band 6 is applied based on initial assessment. Due to the resulting lack of the cloud information, the first two pixels of each scanline cannot be analyzed. The miss-registration might cause an over- or underestimation of the real cloud top altitude. A cloud top height error of 1 km may lead to total ozone errors of up to 1.5%.

Outliers

It has been identified that the product includes some rare outliers with unphysical retrieved effective temperature and total ozone columns. Those pixels are currently not flagged but would be easily removed, if the user use the filters recommended above.

Saturation

Some TROPOMI pixels in band 6 might be affected by saturation. Those pixels should be flagged and their quality is reflected in the `qa_value`. Nevertheless, in the vicinity of saturated pixels there might be pixels also affected by saturation due to the so-called blooming effect. The blooming effect is planned to be corrected for in the future update of the level 1b processor. These pixels cannot be explicitly determined and flagged. This effect is not visible in the band 3 used for total ozone retrievals, but the product may nevertheless be impacted via the cloud parameters. In such cases, the total ozone column values are usually underestimated.

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.

Though this may seem anomalous, it is physically correct, and not related to any problem on the data geolocation.

Metadata/Attributes

The spatial resolution of the TROPOMI measurements is improved by bringing the along track ground pixel size from 7.2 to 5.6 Km starting on 6th August 2019. Note that, after this operations change, the metadata/Attributes fields listed below 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 end of 2019.

4.2 Solved Data Quality Issues

Pressure/AK/Profiles grids (solved in version 01.01.05)

In case of clear cases (cloud fraction=0), there is one layer less in the forward model and the pressure, a-priori profiles and averaging kernels grids are given in an inconsistent way in the output files. This was solved since version 01.01.05 (see Table 2).

Orbit numbering in NRTI and OFFL (solved in version 01.01.05)

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 01.01.05 (see Table 2).

Impact of cloud product (solved in version 01.01.06)

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).

Smoothing error (solved in version 01.01.06)

The smoothing error representing the systematic error estimate due to the usage of the a-priori profile is provided in Dobson Unit instead of mol.cm^{-2}. Values consistent with the other variables are obtained by dividing them by 2241.15. From version 01.01.06 (see Table 2), the unit of this variable is mol.cm^{-2}, consistently with the other variables.

Data gaps at activation of V01.01.06 (solved in version 01.01.07)

Ozone data processed with version 01.01.06 (between 28-03-2019 and 23-04-2019, see Table 2) 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 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.

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__O3____ 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.

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 OFFL total ozone product, therefore there are no changes to report.

7 Product Availability

The S5p OFFL data are available at 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 Operation Phase;
source: ESA; **ref**: ESA-EOPG-CSCOP-PL-0073;
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 Total Column;
source: DLR; **ref**: S5P-L2-DLR-ATBD-400A;
https://sentinels.copernicus.eu/documents/247904/2476257/Sentinel-5P-TROPOMI-ATBD-Total-Ozone

[RD03] Sentinel-5 precursor/TROPOMI Level 2 Product User Manual O3 Total Column;
source: DLR; **ref**: S5P-L2-DLR-PUM-400A;
https://sentinels.copernicus.eu/documents/247904/2474726/Sentinel-5P-Level-2-Product-User-Manual-Ozone-Total-Column

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

AMF	Air Mass Factor
ATBD	Algorithm Theoretical Basis Document
BIRA-IASB	Royal Belgian Institute for Space Aeronomy
CF	Cloud Fraction (fractional cloud cover)
COT	Cloud Optical thickness
CRB	Cloud as Reflecting Boundaries
CTH	Cloud Top Height
DLR	German Aerospace Center / Deutsches Zentrum für Luft- und Raumfahrt
DOAS	Differential Optical Absorption Spectroscopy
DOI	Digital Object Identifier
ESA	European Space Agency
ESL	Expert Support Laboratory
EU	European Union
GB	Ground Based
GOME(-2)	Global Ozone Monitoring Experiment(-2)
KNMI	Royal Netherlands Meteorological Institute / Koninklijk Nederlands Meteorologisch Instituut
MetOp	polar orbiting Meteorological Operational satellite
MPC	Mission Performance Centre
NASA	National Aeronautics and Space Administration
NDACC	Network for the Detection of Atmospheric Composition Change
OMPS	Ozone Mapper and Profiling Suite
PRF	Product Readme File
PUM	Product User Manual
QWG	Quality Working Group
S5p	Sentinel-5 Precursor
S5PVT	Sentinel-5 Precursor Validation Team
Suomi NPP	Suomi National Polar-orbiting Partnership
SZA	Solar Zenith Angle
TROPOMI	Tropospheric Monitoring Instrument
VDAF	Validation Data Analysis Facility
VIIRS	Visible Infrared Imaging Radiometer Suite
WMO	World Meteorological Organization