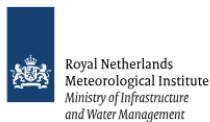




S5P Mission Performance Centre Readme OFFL Total Ozone



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CHANGE LOG

Reason for change	Issue	Revision	Date
Table 2: addition of version 01.01.08	1	6	27/03/2020
Updates for processor version 02.01.03	2	0	16/07/2020

1 Summary

This is the Product Readme File (PRF) for the 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.

Product Identifier: **L2_O3**_____

Example filename:

S5P_OFFL_L2_O3_____20190729T012853_20190729T031221_09274_01_020103_20200520T121402.nc

This product has the following Digital Object Identifier (DOI): <https://doi.org/10.5270/S5P-ft13p57>

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.

As a user guideline for the data quality a `qa_value` is given with the data. In order to avoid misinterpretation of the data quality, it is recommended at the current stage to only use those pixels with `qa_value` above 0.5.

Independent validation by Mission Performance Centre (MPC) Cal/Val experts and the Sentinel-5 Precursor Validation Team (S5PVT) conclude that version 1.x.x of the OFFL 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.

Up to date validation results are available in the Routine Operations Consolidated Validation Reports (ROCVR) that are accessible through the MPC Validation Data Analysis Facility (VDAF) website at <http://mpc-vdaf.tropomi.eu>. The ROCVR reports are issued quarterly, and reports released after July 2020 include validation results based on processor version 2.x.x.

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

Table 1: Ozone Offline data products uncertainty requirements

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
02.01.03	OFFL: orbit14239, 2020-07-13	Current version	<ul style="list-style-type: none"> - New surface albedo retrieval algorithm (GE_LER) from TROPOMI for the CLOUD product (affects CLOUD input product) - New OCRA cloud-free maps based on S5P 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 issues 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 (see section 6.1) - Fixed inconsistency in the surface / effective scene pressure calculation in the O₃ OFFL algorithm - Improve the <code>qa_value</code> determination - Improve the prior value of the effective scene albedo - Fixed inconsistency in the surface/effective scene pressure calculation in the algorithm - Invalid values of <code>geolocation_flags</code> set to correct values - New metadata added (see section 6.1)
01.01.08	OFFL: orbit 12432, 2020-03-07	Orbit14238, 2020-07-12	No changes with respect to previous version
01.01.07	RPRO: orbit 2818, 2018-04-30 OFFL: orbit 7907, 2019-04-23	Orbit 7906, 2019-04-23 Orbit 12431, 2020-03-07	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)

01.01.06	OFFL: orbit 7542, 2019-03-28	Orbit 7906, 2019-04-23	<ul style="list-style-type: none"> - 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 <code>smoothing_error</code> 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
01.01.05	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)
01.01.02	OFFL: orbit 4147, 2018-08-01	Orbit 5832, 2018-11-28	Initial operational version

Table 2: History of Ozone OFFL 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

The quality of the individual observations depends on many factors, including cloud cover, presence of snow-ice, saturation, geometry etc. These aspects are taken into account in the definition of the "quality assurance value" (`qa_value`), available for each individual observation, which provides the users of the data with an easy filter to remove less accurate observations. The `qa_value` is a continuous variable, ranging from 0 (error) to 1 (all is well). It is recommended to only use those TROPOMI pixels associated with a `qa_value` above 0.5. This helps to remove observations with poor quality fits, less favorable geometry observations or with poorer cloud input parameters

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

Independent validation by Mission Performance Centre (MPC) Cal/Val experts and the Sentinel-5 Precursor Validation Team (S5PVT) conclude that version 1.x.x 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 $\pm 2.5\%$.

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

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.

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 Cloud Fraction at Bands 3 and 4 and interpolates it linearly, according to the covered area, to band 6. 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. The cloud height and optical thickness retrieved in band 6 are interpolated back to the band 3 footprints. Due to missing overlap with the band 6 footprints, the first pixel in band 3 (no overlap) and the second pixel in band 3 (only partial overlap), do not contain cloud products with full quality. This is also reflected in the cloud data `qa_value`.

Outliers

It has been identified that the product includes some rare outliers with unphysical retrieved effective temperature and total ozone columns, or poor fit quality (high `fitted_root_mean_square`). Those pixels are in principle removed when using a `qa_value` larger than 0.5.

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.

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.

Metadata/Attributes (solved in version 02.01.03)

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, some metadata/Attributes fields related to the spatial resolution, remained **unchanged** (hence not aligned to the improved resolution).

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.

4.4 Mission Operations Changes

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.

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

6.1.1 New variables

```
/PRODUCT/SUPPORT_DATA/INPUT_DATA/northward_wind  
/PRODUCT/SUPPORT_DATA/INPUT_DATA/eastward_wind  
/PRODUCT/SUPPORT_DATA/INPUT_DATA/sea_ice_cover  
/PRODUCT/SUPPORT_DATA/INPUT_DATA/snow_cover
```

6.1.2 New Metadata

Added "Status_BG" as global attribute.

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
ROCVR	Routine Operations Consolidated Validation Report
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