



S5P Mission Performance Centre NRTI Total Ozone [L2__O3____] Readme



document number	S5P-MPC-DLR-PRF-O3	
issue	2.2	
date	2021-07-05	
product version	V02.02.01	
status	Released	
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¹ The S5PVT AO project summaries can be found at <https://earth.esa.int/web/guest/pi-community/search-results-and-projects/mission>

CHANGE LOG

Reason for change	Issue	Revision	Date
Table 2: addition of version 01.01.08	1	6	18/03/2020
Updates for processor version 02.01.03	2	0	16/07/2020
<ul style="list-style-type: none">Table 2: addition of version 01.01.04Section 3.1: put back the data selection criteria for V1.x.x, as this data are still available	2	1	26/11/2020
<ul style="list-style-type: none">Table 2: adapting to version 02.02.01 of the processorSection 4.1 & section 4.2: some text moved from section 4.1 (Known Data Quality Issues) to section 4.2 (Solved Data Quality Issues)Section 6.1: added format changes related to version 02.02.01	2	2	05/07/2021

1 Summary

This is the Product Readme File (PRF) for the Copernicus Sentinel 5 Precursor Tropospheric Monitoring Instrument (S5P/TROPOMI) Total Ozone Level 2 data product and is applicable for the Near Real Time (NRTI) timeliness product.

Product Identifier: **L2_O3**_____

Example filename:

S5P_NRTI_L2_O3_____20190405T030130_20190405T030630_07643_02_020103_20190405T034612.nc

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 provides the total atmospheric column between the surface and the top of atmosphere. The respective random error originating from the spectral fit is given in the `ozone_total_vertical_column_precision`. 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.

Note: Starting from processor version 2.2.1, new improved Level 1b version 2.0.0 data products are used as input [RD05].

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

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.

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

Table 1: Ozone data product requirement from the S5P Calibration and Validation Plan [RD01]

2 Processing baseline description

Table 2 contains the history of the NRTI Total Ozone processor versions. Note that the processor version for O3 NRTI 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 NRTI product.

Processor Version	In operation from	In operation until	Relevant improvements
02.02.01	Orbit 19308, 2021-07-05	Current version	<ul style="list-style-type: none"> - From this version, the variable <code>surface_altitude_precision</code> is correctly written (previous versions reported fill-value) - New fallback surface albedo climatology based on 3 years of TROPOMI data - Optimized for the new L1b V2.0 input, including updates to the destriping and degradation correction - Improved clear-sky filtering in background correction - Added surface temperature and DOAS polynomial coefficients (see section 6.1) <p>Note: Starting from processor version 2.2.1, new improved Level 1b version 2.0.0 data products are used as input [RD05].</p>
02.01.04	Orbit 16259, 2020-12-02	Orbit 19306, 2021-07-05	No changes with respect to previous version
02.01.03	Orbit 14285, 2020-07-16	Orbit 16256, 2020-12-02	<ul style="list-style-type: none"> - New surface albedo retrieval algorithm (GE_LER) from TROPOMI for the NRTI O3 and CLOUD product replace the climatologies - New OCRA cloud-free maps based on TROPOMI instead of OMI (affects CLOUD input product) - Since this version, SNPP data for UVIS and NIR are ingested and written into the OFFL CLOUD input product - 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 input product - Added spike removal for NRTI O3 - 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, extracting Geopotential at Ground/Water Surface level, and propagating wind-information in the level 2 products (see section 6.1)

			<ul style="list-style-type: none"> - Improved the parameter <code>qa_value</code> determination - Invalid values of <code>geolocation_flags</code> set to correct values - New variables added (see section 6.1)
01.01.08	Orbit 12482, 2020-03-11	Orbit 14285, 2020-07-16	No changes with respect to previous version
01.01.07	Orbit 8000, 2019-04-30	Orbit 12482, 2020-03-11	No changes respect to previous version
01.01.06	Orbit 7632, 2019-04-04	Orbit 7999, 2019-04-30	<ul style="list-style-type: none"> - Correction of occasional Cloud As Layers (CAL) cloud top pressure field too high in Tropical regions that caused the total ozone columns to be biased low (see section 4.2) - Surface classification climatology updated - Fixed a bug in the interpolation of the surface albedo climatology
01.01.05	Orbit 5932, 2018-12-05	Orbit 7631, 2019-04-04	No changes with respect to previous version
01.01.02	Orbit 4243, 2018-08-08	Orbit 5929, 2018-12-05	Variable <code>delta_time</code> was not correctly calculated in previous version (see section 4.2)
01.01.01	Orbit 3947, 2018-07-18	Orbit 4242, 2018-08-08	<ul style="list-style-type: none"> - Solved a problem while computing <code>time_coverage_start</code> and <code>time_coverage_end</code> of a granule overpassing midnight (see section 4.2) - Variable <code>processing_quality_flags</code> was not correctly calculated in previous version
01.00.00	Orbit 3745, 2018-07-04	Orbit 3946, 2018-07-18	Initial operational version

Table 2: History of NRTI Total Ozone processor versions

3 Product Quality

3.1 Recommendations for data usage

The quality of the observations depends on many factors which are taken into account in the definition of the `qa_value`. The `qa_value` is a continuous variable, ranging from 0 (error) to 1 (good quality).

- For data Version 1.x.x: the `qa_value` had still to be optimized, therefore the recommendation is to use, instead, the following selection rules:
 - `ozone_total_vertical_column` out of [0 to 0.45]
 - `ozone_effective_temperature` out of [180 to 260]
 - `fitted_root_mean_square` larger than 0.01
- For data Version 2.x.x onwards: the `qa_value` has been adjusted as to reflect the selection criteria listed above (for V1.x.x) and can be used without any additional selection criteria. Therefore, users are recommended to use TROPOMI pixels associated with a `qa_value` above 0.5.

For further details, data users are encouraged to read the Product User Manual (PUM) [RD03] and Algorithm Theoretical Basis Document (ATBD) [RD02] 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

Independent validation by MPC Cal/Val experts and the S5PVT conclude that the Version 1.x.x of the NRTI ozone data is in good overall agreement with (i) reference measurements collected from global ground-based networks, and (ii) the corresponding satellite data products from GOME-2 and OMPS, and (iii) is compliant with the requirements as defined in the **S5P Calibration and Validation Plan** [RD01], see Table 1. The small bias of roughly +1% found in the data comparisons is well within the mission requirements (see **Note**: Starting from processor version 2.2.1, new improved Level 1b version 2.0.0 data products are used as input [RD05]).

Independent validation by Mission Performance Centre (MPC) Cal/Val experts and the Sentinel-5 Precursor Validation Team (S5PVT) conclude that the NRTI Ozone data is compliant with the requirements as defined in the **S5P Calibration and Validation Plan** [RD01], see Table 1.) of maximum 3.5%. The scatter of the data around this bias also complies with mission requirements of at most 2.5%. Differences between S5p TROPOMI and other satellite data sets over cloudy scenes highlight differences in cloud algorithms.

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 Issues

Currently, the following data quality issues are known, not covered by the quality flags, and should be kept in mind when looking at the Ozone NRTI product itself and also at validation results. Several of the issues listed below will be addressed in next processor versions (as part of the algorithm evolution).

An instrument feature: spatial mis-registration between TROPOMI bands 3-4 and band 6

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 in 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 ROCINN algorithm which works in band 6. Over heterogeneous scenes the mis-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) does not contain cloud data and the second pixel in band 3 (only partial overlap), contains cloud products with reduced quality. This is also reflected in the cloud data `qa_value`. A cloud top height error of 1 km may lead to total ozone errors of up to 1.5%.

4.2 Solved Data Quality Issues

Wrong Sensing dates in metadata (solved in version 01.01.01)

Note that there is a non-systematic problem in the sensing dates around mid-night: the reported dates in the global attributes can be wrong by one day ahead. This issue is solved with the activation of version 01.01.01 mid-July 2018 (see Table 2).

NRTI data gaps northern hemisphere (solved in version 01.01.01)

The NRTI data stream shows data gaps over Kazakhstan, southern part of Russia and Canada due to a miss-configuration of the processing facility. This issue is solved with the activation of version 01.01.01 mid-July 2018 (see Table 2).

Bug in `delta_time` variable (solved in version 01.01.02)

In version 01.01.01 (2018-07-18 until 2018-08-08) the `delta_time` variable might be wrong. The error is usually in the range of less than a minute but in the worst case it might be up to 45 min. It is therefore recommended not to use the time variable (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 solved with the activation of version 01.01.05 (see Table 2).

Impact of cloud product (solved in version 01.01.06)

The NRTI product makes use of the Cloud As Layers (CAL) parameters from the CLOUD operational product. Some occasional outliers have been identified in the CAL Cloud Top Pressure fields (CTP too high) in Tropical regions. For such events, the NRTI 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).

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, the metadata/Attributes fields related to the spatial resolution, remained **unchanged** (hence not aligned to the improved resolution) – but with version 02.01.03 this is corrected.

Surface albedo climatology (solved in version 02.01.03)

The surface albedo climatology has a spatial resolution of $0.5^\circ \times 0.5^\circ$. This resolution seems too coarse compared to the much higher spatial resolution of S5p TROPOMI pixels. As a consequence sometimes the albedo structures are observed in the total ozone columns. Especially in northern regions the albedo climatology sometimes has very few grid cells marked as no snow or ice (reflectivity 0.05) where as the reflectivity is close to unity for the neighboring ones with snow. These structures are one to one observed in the ozone_total_vertical_column data e.g. it increases from 0.138 mol/m^2 to $\sim 0.156 \text{ mol/m}^2$ over an area of $0.5^\circ \times 0.5^\circ$ (Figure 1 left). With the new GE_LER retrieval this issue is solved as the G3_LER map is updated on a daily basis.

The Version 2 total ozone retrieval also agrees better with current datasets. A preliminary comparison to CAMS (Copernicus Atmosphere Monitoring Service) total ozone is shown in Loyola et al. (2020) [RD04].

Metadata values exchanged (solved)

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 since the switch to version 02.00.00 of the Level 1b processor July 2021.

Flagging of Saturation (solved)

Some TROPOMI pixels might be affected by saturation. Those pixels are 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. In such cases the total ozone column values are usually underestimated. The pixels affected by blooming effect have been flagged since version 02.00.00 of the Level 1b processor, operational since July 2021.

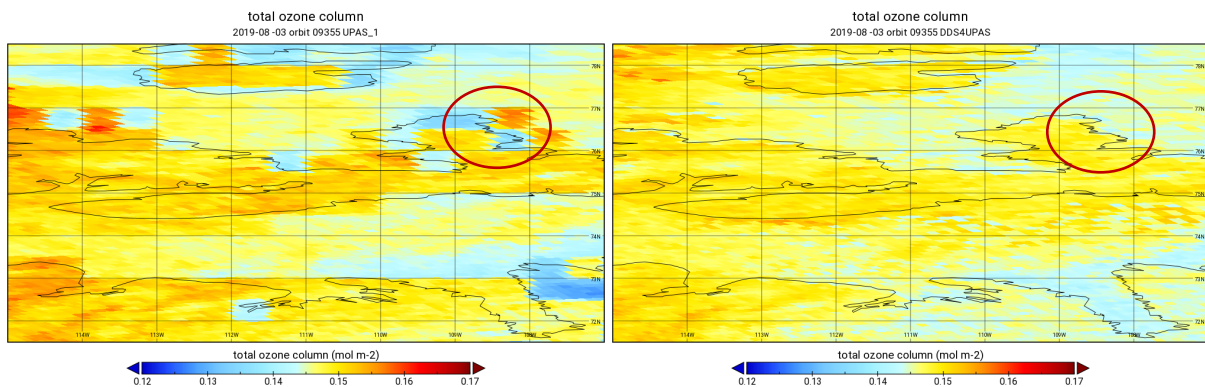


Figure 1: Left: Example over northern Canada ($\sim 75^\circ\text{N}$) of the total ozone outliers (in version 1.x) induced by the albedo climatology, furthermore in some places (e.g. red circle) the 0.5° resolution and the jumps on latitudinal limits of the albedo climatology can be seen. Right: total ozone (in version 2.x) over the same scene using the fitted G3_LER, the ozone column density is much smoother without obvious outliers.

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 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] and Loyola et al. (2020) [RD04].

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.

Please note that consecutive data granules of the NRTI product show an overlap of about 12 scan lines. Details of the data format are provided in the Product User Manual (PUM) [RD03].

6.1 Data format changes

6.1.1 Version 02.02.00

New fields added

```
/PRODUCT/SUPPORT_DATA/INPUT_DATA/surface_temperature  
/PRODUCT/SUPPORT_DATA/DETAILED_RESULTS/number_of_doas_polynomial_coefficients  
/PRODUCT/SUPPORT_DATA/DETAILED_RESULTS/doas_polynomial_coefficients
```

6.1.2 Version 02.01.04

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

6.1.3 Version 02.01.03

New fields added

```
/PRODUCT_SUPPORT_DATA/DETAILED_RESULTS/effective_scene_height  
/PRODUCT_SUPPORT_DATA/DETAILED_RESULTS/effective_scene_height_precision  
/PRODUCT_SUPPORT_DATA/DETAILED_RESULTS/effective_scene_pressure  
/PRODUCT_SUPPORT_DATA/DETAILED_RESULTS/effective_scene_pressure_precision  
/PRODUCT_SUPPORT_DATA/DETAILED_RESULTS/effective_scene_albedo  
/PRODUCT_SUPPORT_DATA/DETAILED_RESULTS/effective_scene_albedo_precision  
/PRODUCT/SUPPORT_DATA/INPUT_DATA/cloud_fraction_apriori  
/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
```

New Metadata

Added "Status_BG" as global attribute.

7 Product Availability

All S5P/TROPOMI data are available on the Copernicus Open Data Hub <https://scihub.copernicus.eu>.

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 Operational Phase
source: ESA; **ref:** ESA-EOPG-CSCOP-PL-0073;
url: <https://sentinel.esa.int/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;
url: <https://sentinel.esa.int/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;
url: <https://sentinel.esa.int/documents/247904/2474726/Sentinel-5P-Level-2-Product-User-Manual-Ozone-Total-Column>
- [RD04] Loyola, D. G., Xu, J., Heue, K.-P., and Zimmer, W.: Applying FP_ILM to the retrieval of geometry-dependent effective Lambertian equivalent reflectivity (GE_LER) daily maps from UVN satellite measurements, Atmos. Meas. Tech., 13, 985–999, <https://doi.org/10.5194/amt-13-985-2020>, 2020.
- [RD05] Algorithm theoretical basis document for the TROPOMI L01b data processor
source: KNMI; **ref:** S5P-KNMI-L01B-0009-SD; **issue:** 9.0.0; **date:** 2019-07-19;
url: <https://sentinels.copernicus.eu/documents/247904/2476257/Sentinel-5P-TROPOMI-Level-1B-ATBD>

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
CTH	Cloud Top Height
DDS	Diagnostic Data Set
DLR	German Aerospace Center / Deutsches Zentrum für Luft- und Raumfahrt
DOAS	Differential Optical Absorption Spectroscopy
ESA	European Space Agency
ESL	Expert Support Laboratory
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
TROPOMI	Tropospheric Monitoring Instrument
VDAF	Validation Data Analysis Facility
VIIRS	Visible Infrared Imaging Radiometer Suite
WMO	World Meteorological Organization