S5P Mission Performance Centre
NRTI Total Ozone [L2__O3_____] Readme

<table>
<thead>
<tr>
<th>document number</th>
<th>S5P-MPC-DLR-PRF-O3</th>
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<tbody>
<tr>
<td>issue</td>
<td>1.6</td>
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<tr>
<td>date</td>
<td>2020-03-18</td>
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<tr>
<td>product version</td>
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<tr>
<td>status</td>
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</table>

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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

<table>
<thead>
<tr>
<th>Reason for change</th>
<th>Issue</th>
<th>Revision</th>
<th>Date</th>
</tr>
</thead>
<tbody>
<tr>
<td>Table 2: addition of version 01.01.08</td>
<td>1</td>
<td>6</td>
<td>18/03/2020</td>
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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.

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.

Product Identifier: L2_O3____
Example filename:
S5P_NRTI_L2_O3____20180710T104700_20180710T105200_03832_01_010000_20180710T113126.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 gives 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.

Independent validation by MPC Cal/Val experts and the Sentinel-5 Precursor Validation Team (S5PVT) conclude that 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 Table 1. The small bias of roughly +1% found in the data comparisons is well within the mission requirements (see Table 1) of maximum 3-4%. The scatter of the data around this bias also complies with mission requirements of ±2.5%. Differences between S5p TROPOMI and other satellite data sets over cloudy scenes highlight differences in cloud algorithms.

The data product requirements are listed in the S5P Calibration and Validation Plan [RD01]

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Data product</th>
<th>Vertical Resolution</th>
<th>Bias</th>
<th>Random</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ozone</td>
<td>Total ozone NRTI</td>
<td>Total column</td>
<td>3.5-5%</td>
<td>1.6-2.5%</td>
</tr>
</tbody>
</table>

Table 1: Ozone data product requirement form 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.

<table>
<thead>
<tr>
<th>Processor Version</th>
<th>In operation from</th>
<th>In operation until</th>
<th>Relevant improvements</th>
</tr>
</thead>
<tbody>
<tr>
<td>01.01.08</td>
<td>Orbit 12482, 2020-03-11</td>
<td>Current version</td>
<td>No changes with respect to previous version</td>
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<tr>
<td>01.01.07</td>
<td>Orbit 8000, 2019-04-30</td>
<td>Orbit 12482, 2020-03-11</td>
<td>No changes respect to previous version</td>
</tr>
</tbody>
</table>
| 01.01.06          | Orbit 7632, 2019-04-04 | Orbit 7999, 2019-04-30 | - 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 delta_time was not correctly calculated in previous version (see section 4.2) |
| 01.01.01          | Orbit 3947, 2018-07-18 | Orbit 4242, 2018-08-08 | - Solved a problem while computing time_coverage_start and time_coverage_end of a granule overpassing midnight (see section 4.2)  
   - Variable processing_quality_flags 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

In order to avoid misinterpretation of the data quality, it is recommended at the current stage to only use those TROPOMI pixels following the selecting rules mentioned in section 4.

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

This section presents a summary of the key validation results obtained by the Validation data Analysis Facility (VDAF) of the S5P Mission Performance Centre (MPC) and by the S5P Validation Team (S5PVT). It contains preliminary results reported at the S5P First Public Release Validation Workshop (ESA/ESRIN, June 25-26, 2018). Individual contributions to the workshop are available in https://nikal.eventsair.com/QuickEventWebsitePortal/sentinel-5p-first-product-release-workshop/sentinel-5p, 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 need to be confirmed by a larger amount of co-locations, and extended over 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. Over the validation period, 20 to 100 co-locations have been identified at about 20 Brewer and Dobson sites and at 11 SAOZ sites, sampling many latitudes from the Arctic to the Antarctic.

3.2.2.2 Satellites

Initial S5P/TROPOMI L2 O3 total ozone column data have also been compared to MetOp-A and B GOME-2 ozone column data (version GDP 4.8), to Suomi-NPP OPMS-nadir ozone column data, and to S5p ozone column data retrieved with the S5p OFFL processor.

3.2.3 Validation results

Overall, the quality of the initial L2 O3 NRTI data product appears to comply with the mission requirements (Table 1): bias of max. 3.5-5% and 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 DLR and BIRA-IASB lead to the following preliminary conclusions:

- **Bias:** the systematic difference between S5p and reference ground-based data at individual stations rarely exceeds 3%, as depicted in Figure 1. The median bias calculated over the entire ground-based networks is of the order of +1%. Between 50’S and 50’N, the mean agreement with other satellite data usually is within 1% as well. This median bias value falls well within the mission requirements (max. bias 3.5-5%).
• **Random difference:** the ±1σ spread of the bias (between S5p and reference data) around its median value rarely exceeds 3-4% 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 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. The scatter of the data comparisons of about 2-4% increases up to 7% at large SZAs beyond 80° and at latitudes beyond 50°.

• **Geographical patterns:** Maps of the bias between S5p and other satellite data sets reveal correlation with weather patterns and atmospheric circulation features. These patterns are likely to be associated with differences in the processing of the cloud properties, and also to differences in overpass times (3.5 hours difference between S5p and GOME-2), although there is a systematic positive difference between S5p and GOME-2 total ozone values in these structures.

• **Short-term variability:** Qualitatively, at all of the 30 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 and ground-based 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 differences. For clarity, sunrise and sunset SAOZ measurements have been offset by -0.5° and +0.5° in latitude.
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.

In addition, the qa_value has still to be optimized, therefore the recommendation is to use the following selection rules until the qa_value covers most uncertainties:

- **ozone_total_vertical_column** out of [0 to 0.45]
- **ozone_effective_temperature** out of [180 to 280]
- **fitted_root_mean_square** larger than 0.01

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 in the order of half a ground pixel. The OCRA algorithm retrieves the CF at Bands 3 and 4. 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. 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 lack of the cloud information the first two pixels of each scanline cannot be analyzed. The mis-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%.

Surface albedo climatology

The current surface albedo climatology has a spatial resolution of 0.5° x 0.5°. 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 0.2 mol/m² to ~0.23 mol/m² over an area of 0.5°x0.5° (Figure 2).

![total ozone column](image)

Figure 2 - Example over northern Canada for the sudden increase in the total ozone column caused by the surface albedo climatology.
Saturation

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.

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.

Metadata/Attributes

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, 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 second half of 2020.

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).

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.

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

There are no changes to report.
7 Product Availability

All S5P/TROPOMI data are available on the Copernicus Open Data Hub [https://scihub.copernicus.eu](https://scihub.copernicus.eu).


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:

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

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
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
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