S5P Mission Performance Centre
NRTI Total Ozone [L2__O3____] Readme

document number	S5P-MPC-DLR-PRF-O3	
issue	1.1	
date	2018-12-04	
product version	V01.01.05	
status	Released	
Prepared by	K.-P. Heue (DLR), T. Verhoelst (BIRA-IASB), J.-C. Lambert (BIRA-IASB),	MPC Product Lead MPC Validation Coordinator MPC ESL-VAL Lead
Reviewed by	J.-C. Lambert (BIRA-IASB), D. Loyola (DLR), J. P. Veefkind (KNMI), A. Dehn (ESA)	MPC ESL-VAL Lead MPC ESL-L2 Lead MPC Technical Manager MPC Technical Officer
Approved by	A. Dehn (ESA), C. Zehner (ESA)	ESA Data Quality Manager ESA Mission Manager

MPC Contributors	G. Granville (BIRA-IASB) C. Lerot (BIRA-IASB) D. Loyola (DLR) F. Romahn (DLR) P. Valks (DLR) M. Van Roozendael (BIRA-IASB) J. Xu (DLR) W. Zimmer (DLR)	MPC ESL-VAL Contributor MPC ESL-L2 Product Coordinator MPC ESL-L2 Lead MPC ESL-L2 Processor Contributor MPC ESL-L2 Product Contributor MPC ESL-L2 Product Contributor MPC ESL-L2 Product Contributor MPC ESL-L2 Processor Lead
S5PVT[1] Contributors	D. Balis (AUTH) A. Bazureau (LATMOS-CNRS) V. Fioletov (ECCC) K. Garane (AUTH) F. Goutail (LATMOS-CNRS) ML. Koukouli (AUTH) C. McLinden (ECCC) A. Pazmiño (LATMOS-CNRS) J.-P. Pommereau (LATMOS-CNRS) C. Zerefos (A.Athens)	S5PVT, VALTOZ Project, AO 28568 S5PVT, VALTOZ Project, AO 28568 S5PVT, ECCC Project, AO 28536 S5PVT, VALTOZ Project, AO 28568 S5PVT, VALTOZ Project, AO 28568 S5PVT, VALTOZ Project, AO 28568 S5PVT, ECCC Project, AO 28536 S5PVT, VALTOZ Project, AO 28568 S5PVT, VALTOZ Project, AO 28568 S5PVT, VALTOZ Project, AO 28568
Signatures	Klaus-Peter Heue Digitally signed by Klaus-Peter Heue DN: C=DE, S=Bavaria, O=DLR, OU=IMF-ATP, CN=Klaus-Peter Heue, E=Klaus-Peter.Heue@DLR.de Location: Oberpfaffenhofen Date: 2019-02-05 13:09:15 Foxit PhantomPDF Version: 9.3.0 X MPC Product Lead / PRF Lead Editor X A. Dehn (ESA) Data Quality Manager Claus Zehner Digitally signed by Claus Zehner Date: 2019.02.04 15:40:39 +01'00' C. Zehner (ESA) – Mission Manager	

[1] The S5PVT AO project summaries can be found at https://earth.esa.int/web/guest/pi-community/search-results-and-projects/mission

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_____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]

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

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.

Processor Version	In operation from	In operation until
01.00.00	Orbit 3745, 2018-07-04	Initial version
01.01.01	Orbit 3947, 2018-07-18	Orbit 4242, 2018-08-08
01.01.02	Orbit 4243, 2018-08-08	Orbit 5929, 2018-12-05
01.01.05	Orbit 5932, 2018-12-05	Current 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.

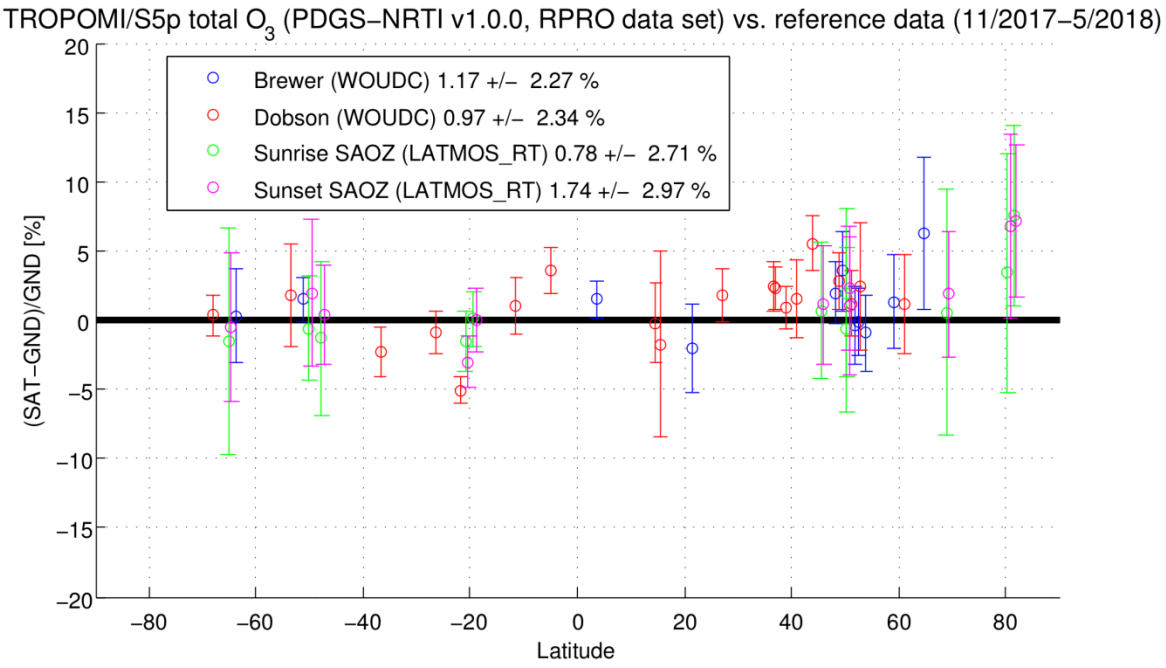

Figure 1 - Meridian dependence of the median and spread (±1 sigma) of the bias between S5p TROPOMI L2_O3 and ground-based reference ozone column data, represented at individual stations from the Antarctic to the Arctic and per reference measurement type (Brewer, Dobson and SAOZ). The values in the legend 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 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 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_columnn` 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).

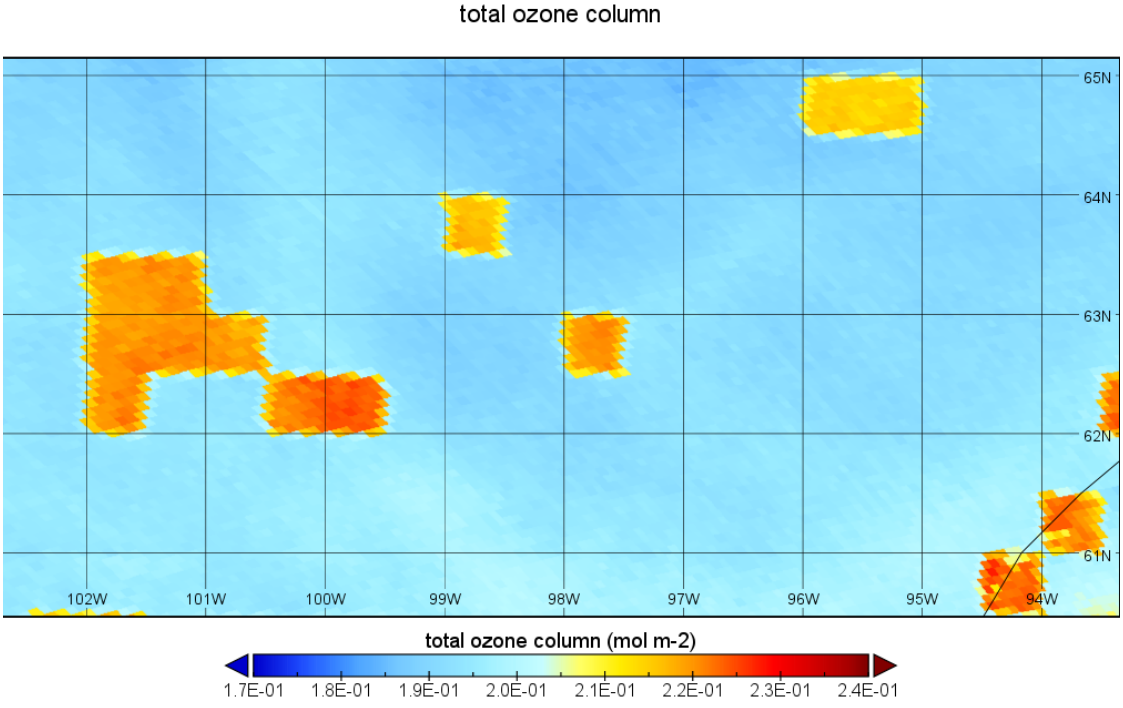

Figure 2 - Example over northern Canada for the sudden increase in the total ozone column caused by the surface albedo climatology.

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.

Wrong Sensing dates in metadata (solved)

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 **01.01.00** mid-July 2018**.**

NRTI data gaps northern hemisphere (solved)

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 **01.01.00** mid-July 2018.

Orbit numbering in NRTI and OFFL (solved)

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** beginning of December 2018.

Bug in `delta_time` variable (solved)

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.

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.

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 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