



S5P Bromine Monoxide [L2__BRO__] [AUX_BGBRO_ [AUX_RARBD3] Readme



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Changelog

Reason for change	Issue	Revision	Date
First draft	0	1	2020-07-22
Update to processor version 1.1.1	1	0	2022-01-22
Update to processor version 1.2.1; Description of S5P-PAL pre-operational environment; Multiple text corrections.	1	1	2022-06-17
Update according to processor version 1.2.3 and the use of L1b Collection 3 data. Several text corrections.	1	2	2023-12-24
Update reflecting patch processor version 1.2.4.	1	2.1	2024-05-02
Bug fix version. Incidentally, ground pixel coordinates are wrongly determined during orbit maneuvers. The qa_value for these pixels is now set to zero (0).	1	2.2	2024-06-08

1 Summary

This is the Product Readme File (PRF) for the Copernicus Sentinel 5 Precursor Tropospheric Monitoring Instrument (S5p/TROPOMI) Total Bromine monoxide Level 2 data product and is applicable for Offline (OFFL) products. The full processor is made up of a main processor, called TCBRO (total column BrO) and an auxiliary processor for the generation of data for background offset correction and the use of radiance data as spectral reference, called BGBRO (background BrO).

Product Identifiers: **L2_BRO**, **AUX_BGBRO**, **AUX_RARBD3**

Example filenames:

S5P_OFFL_L2_BRO____20190330T174932_20190330T193102_07567_03_010303_20231113T051447.nc

S5P_OFFL_AUX_BGBRO__20190921T231149_20190923T003410_20231204T115351

S5P_OFFL_AUX_RARBD3_20191022T232727_20191024T004949_20231204T083952

This Readme file describes the current processing baseline, product and quality limitations, and product availability status.

The data file contains the brominemonoxide_total_vertical_column which gives the total atmospheric column between the surface and top of atmosphere. The random error uncertainty originating from the spectral fit is given in the brominemonoxide_total_vertical_column_precision. Other uncertainty terms are provided in the support_data, as for example the systematic error uncertainties

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 a qa_value above 0.5.

Initial validation exercises show a good agreement with zenith-sky ground-based measurement and with total BrO columns from the GOME-2 instruments on the MetOp-B and -C platforms [RD05].

2 Processing baseline description

The history of the TCBRO processor versions is detailed in Table 1.

Processor Version	Applied from	Applied until	Relevant development
01.02.05 (August 2024)	Patch version correcting a bug related to ground occasional erroneous ground pixel geolocation assignment during orbit maneuvers. The affected pixels sometimes caused problems during orbit visualization or L2 -> L3 gridding operations.		<ul style="list-style-type: none"> - Here geolocation flags indicated erroneous geolocations, the geolocation in latitude_bounds/longitude_bounds is set to NaN. Also, the affected pixels not get assigned qa_value = zero (0).
01.02.04 (May 2024)	This patch version corrects a bug in the calculation of the global file variable time_reference, resulting in main processor TCBRO v1.2.4 and auxiliary processor BGBRO v1.2.3. These versions also saw an update from QDOAS version 3.6.0 to version 3.6.5, which fixes some small bugs and is more memory efficient.		<ul style="list-style-type: none"> - Corrected calculation of time_reference - Upgrade to QDOAS version 3.6.5
01.02.03 (2023)	This version is a technical upgrade, facilitating the installation and operation of the code both on PAL and offline linux environments. The current L2 data available from the PAL pre-operational environment will gradually be replaced by data from this latest processor version early 2024.		<ul style="list-style-type: none"> - Revised installation procedure. - Use of conda-forge package of QDOAS v3.6. - Multiple small error corrections in L2 output file format.
01.02.01	This version of the processor is active in the S5P-PAL pre-operational environment. Newly arriving L1b data is automatically processed. L2 data from the beginning of the S5P mission to the processor activation date will gradually be made available over the next months.		<ul style="list-style-type: none"> - File format corrections of inconsistent variable/attribute types. - Introduction of the dynamic 'PAL_' file class, - Minor changes to the preliminary error budget calculations.
01.01.01	OFFL: orbit 6309 2019-01-01	OFFL: orbit 11452 2019-12-31	Output file attribute data type corrections.
01.01.00 July 2021	OFFL: orbit 6309 2019-01-01	OFFL: orbit 11452 2019-12-31	All components in place. First full netCDF4 output file format. Proper ingestion of BGBRO auxiliary processor data.
00.01.00 July 2020	OFFL: orbit 6309 2019-01-01	OFFL: orbit 11452 2019-12-31	Initial version. Temporary output format as HARP netCDF4.

Table 1: History of TCBRO/BGBRO processor versions

3 Product Quality

3.1 Recommendations for data usage

In order to avoid misinterpretation of the data quality, it is recommended to only use those TROPOMI pixels associated with a quality assessment value (qa_value) above 0.5. The qa_value is a continuous variable, ranging from 0 (error) to 1 (good quality). While it is a handy way of filtering observations of low quality, the “quality assurance value” should also be considered with caution, as it is a compromise to take into account several aspects that may affect the product result. Currently, pixels are considered of good quality if:

- The solar zenith angle is not too large (certainly below 89 degrees, but preferably < 75 degrees).
- The fitting RMS < 2×10^{-3} .
- The BrO vertical column is a valid number.

Further flagging refinement may be applied in the future.

For details regarding the qa_value and its location in the product files, see [RD02], [RD01], and [RD03].

Remark: L2 version 1.2.3 fixes a bug where the qa_value was set to 1.0 in case of missing cloud parameters.

3.2 Validation results

Initial validation results performed at BIRA-IASB for 2019 concludes that the TROPOMI bromine monoxide column is in good overall agreement with (i) reference measurements collected from ground-based zenith-sky measurements and, and (ii) the corresponding satellite data products from GOME-2 (-B and -C).

In comparisons for 12 overpass sites, a positive bias of 0 - 50% is observed with respect to the GOME-2 instruments, depending on measurement time and location. It is thought that this is at least in part due to a negative offset in the GOME-2 measurements ([RD05]). Another component in the deviation is likely caused by the geometric approach for the AMF in TCBRO. More detailed studies of the offsets as function of measurement time and observed seen should give better insight in this phenomenon.

The agreements of the TCBRO columns with Harestua zenith-sky measurements is very good with an overall offset of -6 ± 12 % over the full year 2019 and -0.2 ± 9 % for the time frame March – October.

More comparisons with independent data sets are expected to be performed in the future.

4 Data quality remarks

4.1 Known Data Quality Issues

AMF-related issues

No specific data quality issues are known at the moment. However, the TCBRO algorithm currently applies a geometric AMF and certain known issues from other product may apply that are related to AMF aspects. Further analysis in the future of physical components that contribute to the AMF may be ground for further algorithm development and refinement of the quality flagging in the BrO L2 product.

Background correction

The determination of the TCBRO BrO columns relies on background correction information and the use of radiance data as reference spectrum in the fit procedure. This information is determined on a daily basis by the BGBRO auxiliary processor and for the BrO retrieval the BGBRO information for the day closest in time to the measurements is adopted. If no suitable data is found, no processing is performed.

Negative slant columns

Because of noise on the data, negative vertical column values are often observed in particular over clean regions or for low BrO emissions. It is recommended not to filter these values except for clear outliers.

4.2 Corrected data quality issues.

Upon processor version updates, corrected data quality issues will be listed here.

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 the 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 Change

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 from 6 August 2019, orbit 9388.

5 Algorithm Change Record

For a detailed description of the L2__TCBRO__ algorithm, please refer to the ATBD [RD01].

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. Processing of near-real time (NRTI) data the product is currently not foreseen.

Details of the data format are provided in the Product File Specification document ([RD02]) and in the Product User Manual (PUM) [RD02].

6.1 Data format changes

Since the first draft of this document, the file format changed from a HARP-compliant netCDF4 file structure ([ER01]) to a netCDF4 structure with content organized according to the S5P-PAL guidelines ([RD04]).

In processor version 01.02.00, a file class 'PAL_' was introduced. This replaces the file class 'OFFL' when the L1B > L2 processing takes place on the S5P-PAL system. This is reflected in the resulting output files through the 'file_class' global attribute and through the output file name, where 'OFFL' is replaced by 'PAL_'.

The latest L2 product version, saw merely technical updates and is applied to Collection 3 of the L1b spectral data.

7 Product Availability

The latest product release, version 01.02.04, is available for download from the data portal ([ER03]) of the so-called pre-operational environment of the S5P-PAL system ([ER02]).

The data can be downloaded on a per-orbit basis through the interactive file browser or programmatically through the API of the STAC archiving system used by the PAL.

8 References

- [RD01] Sentinel-5 precursor/TROPOMI Level 2 Algorithm Theoretical Basis Document Total Bromine Monoxide, **source:** BIRA; **ref:** S5P- BIRA-L2- ATBD-TCBRO; **issue:** 1.2.0; **date:** 2023-12-23.
- [RD02] Sentinel-5 precursor/TROPOMI Level 2 Product User Manual TCBRO, **source:** BIRA; **ref:** S5P-L2-BIRA-PUM-TCBRO; **issue:** 1.2.0; **date:** 2023-12-23.
- [RD03] S5P/TROPOMI Level 2 Product Format Specification for the offline Total Bromine Monoxide algorithm TCBRO and its auxiliary algorithm BGBRO, **source:** BIRA; **ref:** S5P-L2-BIRA-PFS-TCBRO; **issue:** 1.2.0; **date:** 2023-12-23.
- [RD04] S5p Product Algorithm Laboratory L2 Processor File Format Guidelines. **source:** S&T; **ref:** ST-ESA-S5P_PAL-L2FFG-001; **issue:** 1.4; **date:** 2023-03-27.
- [RD05] S5P/TROPOMI Total BrO Algorithm TCBRO Validation Report. **source:** BIRA; **ref:** S5P-BIRA-L2-TCBRO-VR; **issue:** 1.0.0; **date:** 2022-01-09
- [ER01] <https://atmospherictoolbox.org/harp/>
- [ER02] <https://www.s5p-pal.com/>
- [ER03] <https://data-portal.s5p-pal.com/>

Abbreviations and acronyms

ATBD	Algorithm Theoretical Basis Document
BIRA-IASB	Royal Belgian Institute for Space Aeronomy
ESA	European Space Agency
GOME(-2)	Global Ozone Monitoring Experiment(-2)
IUP-UB	Institute of Environmental Physics – University of Bremen
MAX-DOAS	Multi Axis Differential Optical Absorption Spectroscopy
MetOp	polar orbiting Meteorological Operational satellite
PFS	Product Format Specification
PRF	Product Readme File
PUM	Product User Manual
S5P	Sentinel-5 Precursor
TROPOMI	Tropospheric Monitoring Instrument