



s[&]t

S5P/TROPOMI Level 2 Product User Manual Total Bromine Monoxide TCBRO



sentinel-5p

document number: S5P- BIRA-L2-PUM-TCBRO

CI identification : TBD
issue : 1.1.0
reference : 1.2.1
processor version
date : 2022-06-17
status : Draft

Document approval record

	digital signature
prepared:	Jeroen van Gent
Checked:	
approved PI:	
approved PM:	

Document change record

issue	date	item	comments
0.1.0	2020-07-24	All	Initial draft version
1.0.0	2022-01-12	All	First full version
1.10	2022-04-19		Update that reflects the changes relevant to processor version 1.2.1.

Contents

Document approval record.....	2
Document change record	3
Contents4	
List of figures	5
1 Introduction.....	6
1.1 Identification.....	6
1.2 Purpose and objective	6
1.3 Document overview	6
2 Applicable and reference documents	7
2.1 Applicable documents.....	7
2.2 Standard documents	7
2.3 Reference documents	7
2.4 Electronic references.....	7
3 Terms, definitions and abbreviated terms.....	8
3.1 Terms and definitions	8
3.2 Acronyms and abbreviations.....	8
4 Introduction to the S5P/TROPOMI L2 TCBRO BrO Product.....	9
5 Description of the TCBRO product	11
5.1 Data L2 product file example	11
5.2 General L2 product file content structure.....	12
5.3 Recommendations for using the L2 BrO product.....	13
References	14

List of figures

Figure 1: Enhance BrO concentrations during Arctic spring (April 2019) over high latitude sea ice surfaces (so-called bromine explosion).....	9
Figure 2: Example of a TCBRO L2 Product internal file structure.....	12

1 Introduction

1.1 Identification

This document describes the technical characteristics of the S5p/TROPOMI Level 2 bromine monoxide product that are needed for efficient and correct use of the data contained. This product user manual is specific for product version 1.2.1.

1.2 Purpose and objective

The Sentinel-5 Precursor (S5p) mission is a low Earth orbit polar satellite system that provides information on air quality, climate and the ozone layer. The mission is part of the Global Monitoring of the ESA/European Commission COPERNICUS programme and consists of a satellite platform, the TROPOspheric Monitoring Instrument (TROPOMI) payload, and a ground system. A peer-reviewed publication on the mission can be found in [RD1].

The algorithms for the TROPOMI raw data treatment (L0 – L1b) and the actual L2 data processing are each described in an algorithm theoretical basis document (ATBD). This Product User Manual (PUM) describes the technical characteristics of the S5p/TROPOMI Level 2 geophysical data products produced by TCBRO (Total Column BrO), an algorithm that derives total vertical column densities from TROPOMI measurements. The document contains information for efficient and correct use of the data contained in the TCBRO product files.

1.3 Document overview

Chapter 2 lists applicable and reference documentation relevant to this product. Chapter 3 gives an overview of terms, definitions and abbreviations. Chapter 4 describes the TCBRO L2 product. Chapter 5 lists the structure of S5P/TROPOMI L2 files.

2 Applicable and reference documents

2.1 Applicable documents

- [AD01] S5P – Tailoring of ECSS Standards for the Level 2 Processor Development; source: ESA; ref: SP-RS-ESA-GS-055; issue 1.1dr; date: 2012-10-31
- [AD02] Earth Observation Ground Segment File Format Standard, ref: PE-TN-ESA-GS-001, issue: 2.0
- [AD03] S5P_PAL L2 Processor File Format Guidelines, source: S&T, ref: ST-ESA-S5P_PAL-L2FFG-001, issue: 1.3, date: 94-01-2022

2.2 Standard documents

There are no standard documents

2.3 Reference documents

- [RD01] J. P. Veefkind, I. Aben, K. McMullanet al.; TROPOMI on the ESA Sentinel-5 Precursor: A GMES mission for global observations of the atmospheric composition for climate, air quality and ozone layer applications. *Remote Sens. Environ.*, 120(2012), 70; 10.1016/j.rse.2011.09.027.ref: S5P-KNMI-L01B-0004-LI; issue: 3.0.0; date: 2013-11-08
- [RD02] Terms, and symbols in the TROPOMI Algorithm Team; source: KNMI; ref: SN-TROPOMI-KNMI-L2-049-MA; issue: 1.0.0; date: 2015-07-16
- [RD03] S5P/TROPOMI Total BrO Algorithm TCBRO ATBD; source: BIRA-IASB; ref: S5P- BIRA-L2-ATBD-TCBRO, issue: 1.1.0; date: 2022-06-17

2.4 Electronic references

- [URL01] <https://atmospherictoolbox.org>
- [URL02] <http://www.giss.nasa.gov/tools/panoply/>

3 Terms, definitions and abbreviated terms

Terms, definitions and abbreviated terms that are used in the development program for the TROPOMI L0-1b data processor are described in [RD01]. Terms, definitions and abbreviated terms that are used in the development program for the TROPOMI L2 data processors are described in [RD02]. Terms, definitions and abbreviated terms that are specific for this document can be found below.

3.1 Terms and definitions

The most important symbols related to the data product described in this document – some of which are not in [RD02] – are the following:

M	Air mass factor
M_{geo}	geometric air mass factor
N_s	slant column density
N_v	vertical column density

3.2 Acronyms and abbreviations

AMF	Air Mass Factor
BrO	Bromine Monoxide
DOAS	Differential Optical Absorption Spectroscopy
OFFL	Offline
NRT	near-real time (i.e. processing within 3 hours of measurement)
S5P	Sentinel-5 Precursor
S5P-PAL	S5P Product Algorithm Laboratory
SZA	Solar Zenith Angle
TCBRO	Total Column BrO retrieval algorithm
TROPOMI	Tropospheric Monitoring Instrument
VZA	Viewing Zenith Angle

4 Introduction to the S5P/TROPOMI L2 TCBRO BrO Product.

Bromine (Br) plays an important role in atmospheric chemistry in an extended vertical range, from the surface to well into the stratosphere. In the troposphere, the effect of the chemistry of inorganic bromine ($\text{Br} + \text{BrO} + \text{BrONO}_2 + \text{HOBr} + \text{HBr} + \text{BrCl}$) is most noticeable in polar spring, when BrO is released over sea ice-covered regions through a series of heterogeneous photochemical reactions (see e.g. Simpson et al., 2007 and Figure 1). This mechanism depletes tropospheric and boundary layer ozone, changes the oxidizing capacity of the atmosphere and facilitates the deposition of mercury into wild ecosystems. On a more local scale, BrO has been identified over salt deserts and lakes (Hebestreit et al., 1999) and in volcanic plumes (Bobrowski et al., 2003). Also, a variety of observations have shown that inorganic bromine may be produced and sustained in the free troposphere at the global scale.

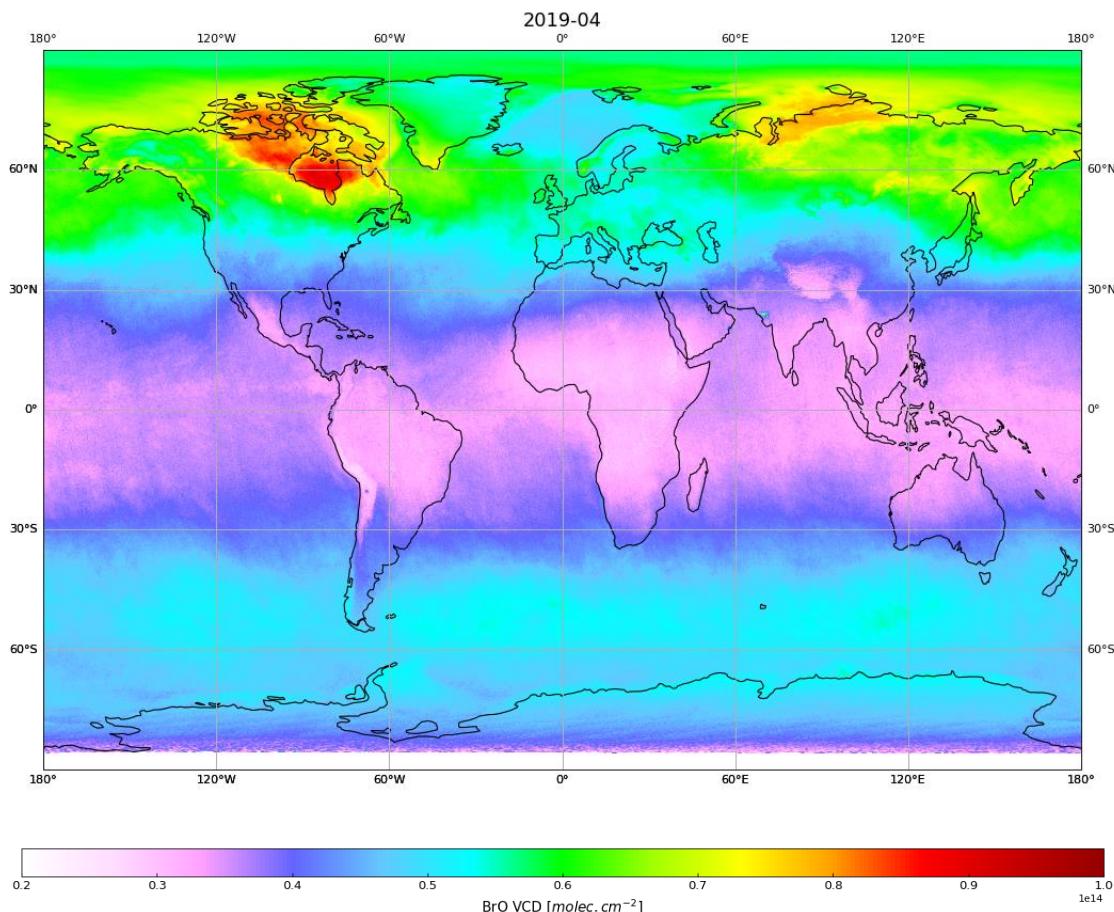


Figure 1: Enhanced BrO concentrations during Arctic spring (April 2019) over high latitude sea ice surfaces (so-called bromine explosion).

Over the last two decades, satellite UV-visible remote sensing observations of BrO have been developed and refined, motivated by their unique capability to study and monitor BrO at the global scale (Chance, 1998; Richter et al., 1997, 2002; Van Roozendael et al., 2002; Wagner and Platt, 1998; Theys et al., 2009; Theys et al., 2011; Sihler et al., 2012; Choi et al., 2018; Seo et al., 2019). This has helped to understand and monitor the evolution of atmospheric bromine and its interaction with a changing climate.

Remote sensing measurements of BrO are generally performed by applying Differential Optical Absorption Spectroscopy (DOAS, Platt & Stutz, 2008), using a fitting window strategically chosen somewhere in the 319-364 nm spectral region, where the molecule exhibits characteristic absorption structures. The retrieved quantity from the spectral fit is a slant column, representing the total BrO density along the integrated light path. This slant column is subsequently converted into a vertical column amount by means of an air mass factor.

The TCBRO algorithm for the derivation of total vertical BrO column densities, was developed in the frame of the ESA-funded project S5P-PAL (Sentinel 5 Precursor Product Algorithm Laboratory). Currently at version 1.2.1, its full details can be found in an Algorithm Theoretical Baseline Document [RD03].

5 Description of the TCBRO product

The current operational S5P L2 products are for the majority formatted according to the guidelines specified in ‘Tailoring of the Earth Observation File Format Standard for the Sentinel 5 precursor Ground Segment’ [AD01], which in turn is based on the ‘Ground Segment File Format Standard’ [AD02]. Products developed within the S5P_PAL have the option to structure their product file content format according to a slightly simplified format, described in [AD03]. The TCBRO L2 product files follow these guidelines. For the file naming, the guidelines from [AD01] are used.

5.1 Data L2 product file example

The output files are in NetCDF-4 format, following the CF convention, and have the ‘.nc’ file extension. The filename of a typical TCBRO L2 output file is structured as follows:

S5P_{OFFL,PAL}_L2_BRO____20191017T232139_20191018T010308_10422_01_010101_20211206T010333.nc

Here, the offline character is indicated by the ‘OFFL’ substring. To discriminate between files produced on the S5P-PAL and the S5P ground segment, the ‘OFFL’ field is replaced by ‘PAL_’ when the file is generated on S5P-PAL. The three date-time fields represent the start and end times of the orbit’s measurements and the file creation time, respectively. The Measurement end time is followed by the orbit number, a collection number inherited from the L1b file and the version number of the L2 algorithm that produced the file.

Every S5P L2 BrO file corresponds to a single orbit of measurements. The detailed file content comprises a wide range of data and metadata variable, including:

- The BrO vertical column, slant column, and air mass factor.
- Time and geolocation (pixel corners and center), inherited from the corresponding L1b product file.
- Retrieval diagnostic parameters, such as uncertainty information and quality flags.
- Input parameters.

5.2 General L2 product file content structure.

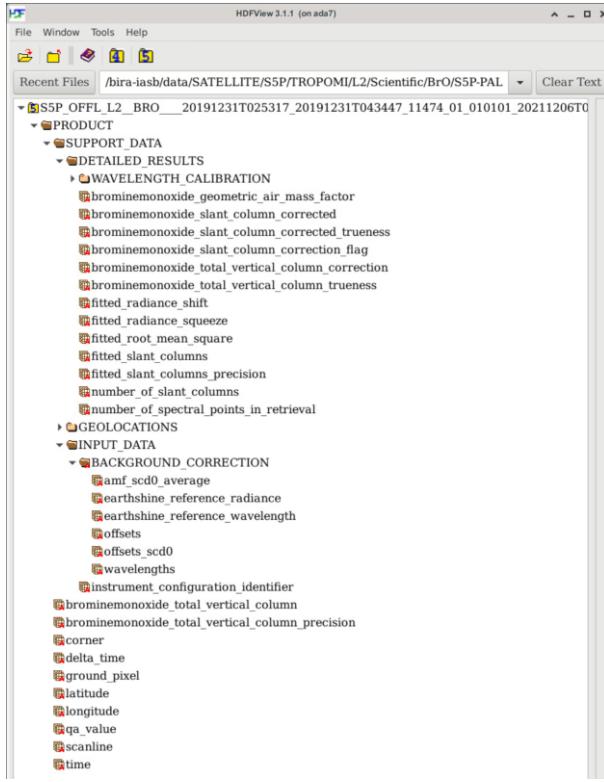


Figure 2: Example of a TCBRO L2 Product internal file structure.

A visualization of the BrO L2 file structure is given in Figure 2. As a high level description, the L2 file are structured as follows:

PRODUCT: This group stores the main data fields of the product, including the precision of the main parameter, latitude, longitude and variables to determine the observation time. The “qa_value” parameter provides an estimate of the reliability of the measurement and range from 100 (high quality) to 0 (poor quality).

SUPPORT_DATA: This group stores additional data needed for advanced use of the product. This group is split into different subgroups:

DETAILED_RESULTS: Additional output, including full state-vectors, error estimates, a priori information, intermediate results...

WAVELENGTH_CALIBRATION: Details regarding the wavelength calibration and shift/stretch procedure.

GEOLOCATIONS: Additional geolocation and geometry related fields, including the pixel corner coordinates, viewing and solar zenith angles, azimuth angles.

INPUT_DATA: Additional input data, such as surface albedo and altitude, cloud information, additional flags...

BACKGROUND_CORRECTION: information related to the equatorial background correction parameters (see also the description in [RD03]).

A full detailed description of all groups and variables can be found in

5.3 Recommendations for using the L2 BrO product.

As mentioned before, the file format is netCDF-4, which is now a standard for Earth Observation missions. This format is versatile, flexible and permits the user to use netCDF-4 or HDF-5 APIs written in many data-analysis packages (e.g. IDL, MatLab, Python, C, C++, ...) in order to read the data. This format also facilitates the visualization of the Geo-2D variables contained in the file as nowadays several tools exist aimed at this purpose, like Panoply [URL02]. Tools for further processing of the data, like filtering, gridding, and comparison are, for example provided through the ESA Atmospheric Toolbox [URL01].

In the L2 product, no filtering was applied for high solar zenith angles (SZA), where product quality tend to be reduced. Nor was any default filter applied to account for reduced fit quality. It is advised the user takes only data pixels into consideration that have a quality value (qa_value in the main PRODUCT group) of 0.5 or higher. This should remove pixels with large SZA or low fit quality. This approach was taken so expert users can decide upon their own filtering method.

References

Bobrowski, N., Hönninger, G., Galle, B., and Platt, U.: Detection of bromine monoxide in a volcanic plume, *Nature*, 423, 273–276, 2003.

Chance, K. and R. J. Spurr: Ring effect studies: Rayleigh scattering including molecular parameters for rotational Raman scattering, and the Fraunhofer spectrum, *Applied Optics*, 36, 5224-5230, 1997.

Choi, S., Theys, N., Salawitch, R.J., Wales, Joiner, J., P.A., Carty, T.P., Chance, K., Suleiman, R., Palm, S.P., Cullather, R.I., Darmenov, A.S., da Silva, A., Kurosu, T.P., Hendrick, F., Van Roozendael,M.: Link between Arctic tropospheric bromine explosion and sea salt aerosols from blowing snow investigated using NASA's Aura Ozone Monitoring Instrument (OMI) BrO data and GEOS-5 model, *J. Geophys. Res. Atmos.*, 123, 2018. <https://doi.org/10.1029/2017JD026889>.

Hebestreit, K., Stutz, J., Rosen, D., Matveiv, V., Peleg, M., Luria, M., and Platt, U.: DOAS measurements of tropospheric bromine oxide in mid-latitudes, *Science*, 283, 55–57, 1999

Platt, U and Stutz, J.: Differential Optical Absorption Spectroscopy: Principles and Applications (Physics of Earth and Space Environments), Springer-Verlag, Berlin, Heidelberg, ISBN 978-3540211938, 2008.

Simpson, W. R., von Glasow, R., Riedel, K., Anderson, P., Ariya, P., Bottenheim, J., Burrows, J., Carpenter, L. J., Frieß, U., Good- site, M. E., Heard, D., Hutterli, M., Jacobi, H.-W., Kaleschke, L., Neff, B., Plane, J., Platt, U., Richter, A., Roscoe, H., Sander, R., Shepson, P., Sodeau, J., Steffen, A., Wagner, T., and Wolff, E.: Halogens and their role in polar boundary-layer ozone depletion, *Atmos. Chem. Phys.*, 7, 4375–4418, doi:10.5194/acp-7- 4375-2007, 2007

Richter, A , F. Wittrock, M. Eisinger and J. P. Burrows (1998), GOME observations of tropospheric BrO in Northern Hemispheric spring and summer 1997, *Geophys. Res. Lett.*, No. 25, pp. 2683-2686.

Richter, A., Wittrock, F., Ladstätter-Weissenmayer, A., and Burrows, J. P. (2002), GOME measurements of stratospheric and tropospheric BrO, *Adv. Space Res.*, 29, 1667-1672.

Seo, S., Richter, A., Blechschmidt, A.-M., Bougoudis, I., and Burrows, J. P.: First high-resolution BrO column retrievals from TROPOMI, *Atmos. Meas. Tech.*, 12, 2913–2932, <https://doi.org/10.5194/amt-12-2913-2019>, 2019

Sihler, H., Platt, U., Beirle, S., Marbach, T., Kühl, S., Dörner, S., Verschaeve, J., Frieß, U., Pöhler, D., Vogel, L., Sander, R., and Wagner, T.: Tropospheric BrO column densities in the Arctic derived from satellite: retrieval and comparison to ground-based measurements, *Atmos. Meas. Tech.*, 5, 2779–2807, <https://doi.org/10.5194/amt-5-2779-2012>, 2012.

Theys, N., Van Roozendael, M., Errera, Q., Hendrick, F., Daerden, F., Chabriat, S., Dorf, M., Pfeilsticker, K., Rozanov, A., Lotz, W., Burrows, J.P., Lambert, J.-C., Goutail, F., Roscoe, H.K., and De Mazière, M.: A global stratospheric bromine monoxide climatology based on the BASCOE chemical transport model, *Atmos. Chem. Phys.*, 9, 831-848, 2009.

Theys, N., Van Roozendael, M., Hendrick, F., Yang, X., De Smedt, I., Richter, A., Begoin, M., Errera, Q., Johnston, P. V., Kreher, K., and De Mazière, M. (2011), Global observations of tropospheric BrO columns using GOME-2 satellite data, *Atmos. Chem. Phys.*, 11, 1791-1811.

Van Roozendael, M., V. Soebijanta, C. Fayt, and J.-C. Lambert: Investigation of DOAS Issues Affecting the Accuracy of the GDP Version 3.0 Total Ozone Product, in ERS-2 GOME GDP 3.0 Implementation and Delta Validation, ERSE-DTEX-EOAD-TN-02-0006, ESA/ESRIN, Frascati, Italy, Chap.6, pp.97-129, 2002.

Wagner, T. and Platt, U.: Satellite mapping of enhanced BrO concentrations in the troposphere, *Nature*, 395, 486–490, <https://doi.org/10.1038/26723>, 1998.

Appendix A – Detailed BrO L2 product file structure

Global attributes

Name	Value	Description
Conventions	"CF-1.7"	CF (Climate and Forecast) conventions used for this product.
Institution	"BIRA-IASB"	Institution responsible for the processing.
source	"Sentinel 5 precursor, TROPOMI, space-borne remote sensing, L2"	Fixed value.
history	"{YYYY-MM-DDThh:mm:ssZ} {executable} {arguments}"	Time of file creation in format "YYYY-MM-DDThh:mm:ssZ" and processor execution.
summary	"TROPOMI/S5P BrO L2 Swath 5.5x3.5km"	Fixed for this product.
id	S5P_{OFFL,PAL}_{L2}_TCBRO_{YYYYMMDDThhmmss}_{YYYYMMDDThhmmss}_{oooooo}_{cc}_{pppppp}_{YYYYMMDDThhmmss}	File id containing measurement start, stop, and file creation date/time. See also [AD02].
time_reference	"{YYYY-MM-DDThh:mm:ssZ}"	Start of the day of sensing time.
collection_identifier	"{xx}"	Two character collection number. Same as is included in the filename. Example: "01"
time_coverage_start	"{YYYY-MM-DDThh:mm:ss.fffZ}"	Start time of first measurement, to millisecond precision.

time_coverage_end	“{YYYY-MM-DDThh:mm:ss.fffZ}”	Start time of last measurement, to millisecond precision.
Time_coverage_resolution	“PT{duration}S”	Duration of scanline in seconds
orbit	nnnnn	Orbit number
processor name	“TCBRO”	Name of the processor
processor_version	“{xx.yy.zz}”	Processor version
processing_center	“{Processing_Station}”	Name of institution where the processing has taken place.
file_class	“OFFL” or “PAL_” (when produced on the S5P-PAL system).	Indicates offline product
footprint	“{GeoJson string}”	Footprint of orbit as GeoJson string
input_files	[“aa.ea”, “bb.eb”, ...]	String containing a list of all input files to the processor

Group structure

The L2 file contains one top-level group, called PRODUCT, and several subgroups. The group structure is outlined below.

Group name	Depth	Description
PRODUCT	0	Contains the main output variables and dimensions.
SUPPORT_DATA	1	Contains only sub groups.
DETAILED_RESULTS	2	Sub group of SUPPORT_DATA. Contains additional outputs, such as slant columns of all fitted species.
WAVELENGTH_CALIBRATION	3	Subgroup of DETAILED_RESULTS. Contains parameters related to the wavelength calibration procedure performed during the slant column fitting.
GEOLOCATIONS	2	Sub group of SUPPORT_DATA. Lists all parameters related to observation geometry and geo-location.

INPUT_DATA	2	Sub group of SUPPORT_DATA. Contains all parameters that the TCBRO algorithm needs as input.
BACKGROUND_CORRECTION	3	Sub group of INPUT_DATA. Lists parameters generated by the BGBRO auxiliary processor and ingested by TCBRO for background correction purposes.

The PRODUCT group

The PRODUCT group is the top-level group and contains the main output variables and dimensions.

Variables in group /PRODUCT:

Variable	Type	Dimensions	Unit	Description
Attribute name	Attribute type	Attribute value		
brominemonoxide_total_vertical_column				
NC_FLOAT	(time, scanline, ground_pixel)	mole m ⁻²	BrO	total vertical column density.
coordinates	NC_CHAR	"/PRODUCT/longitude /PRODUCT/latitude"		
long_name	NC_CHAR	"vertical column of formaldehyde"		
multiplication_factor_to_convert_to_DU	NC_FLOAT	2241.15		
multiplication_factor_to_convert_to_molecules_percm2	NC_FLOAT	6.02214E19		
standard_name	NC_CHAR	"atmosphere mole content of bromine dioxide"		
units	NC_CHAR	"mol m ⁻² "		
brominemonoxide_total_vertical_column_precision				
NC_FLOAT	(time, scanline, ground_pixel)	mole m ⁻²	BrO	total vertical column density random uncertainty
coordinates	NC_CHAR	"/PRODUCT/longitude /PRODUCT/latitude"		
long_name	NC_CHAR	"random error of vertical column density"		
multiplication_factor_to_convert_to_DU	NC_FLOAT	2241.15		
multiplication_factor_to_convert_to_molecules_percm2	NC_FLOAT	6.02214E19		
standard_name	NC_CHAR	"atmosphere_mole_content_of_bromine_monoxide_standard_error"		

units	NC_CHAR	"mol m-2"	
delta_time			
NC_INT	(time, scanline)	milliseconds	Offset from reference start time of measurement
long_name	NC_CHAR	"offset from reference start time of measurement"	
units	NC_CHAR	"milliseconds since {YYYY-MM-DD 00:00:00}"	
latitude			
NC_FLOAT	(time, scanline, ground_pixel)	degree	Center latitude of ground pixel
bounds	NC_FLOAT	"/PRODUCT/SUPPORT_DATA/GEOLOCATIONS/latitude_bounds"	
long_name	NC_CHAR	"pixel center latitude"	
standard_name	NC_CHAR	"latitude"	
units	NC_CHAR	"degrees_north"	
valid_min	NC_FLOAT	-90.	
valid_max	NC_FLOAT	90.	
longitude			
NC_FLOAT	(time, scanline, ground_pixel)	degree	Center longitude of ground pixel
bounds	NC_FLOAT	"/PRODUCT/SUPPORT_DATA/GEOLOCATIONS/longitude_bounds"	
long_name	NC_CHAR	"pixel center longitude"	
standard_name	NC_CHAR	"longitude"	
units	NC_CHAR	"degrees_east"	
valid_min	NC_FLOAT	-180.	
valid_max	NC_FLOAT	180.	
qa_value			
NC_UINT	(time, scanline, ground_pixel)		Quality
add_offset	NC_float	0.	
comment	NC_CHAR		

coordinates	NC_CHAR	"A continuous quality descriptor, varying between 0 (no data) and 1 (full quality data). Recommend to ignore data with qa_value < 0.5"
long_name	NC_CHAR	"/PRODUCT/longitude /PRODUCT/latitude"
scale_factor	NC_FLOAT	"data quality value"
units	NC_CHAR	0.01
valid_max	NC_UNIT	1"
valid_min	NC_UINT	0
		1

Dimension variables in group /PRODUCT:

Name	Type	Size	Unit	Description
Attribute name	Attribute type	Attribute value		
corner				
NC_FLOAT	(4)	1		Pixel corner dimension
comment				
long_name	NC_CHAR			"This coordinate variable defines the indices for the pixel corners; index starts at 0 (counter-clockwise, starting from south-western corner of the pixel in ascending part of the orbit)."
units	NC_CHAR			"pixel corner index"
				"1"
ground_pixel				
NC_INT	(450)			Across-track pixel index dimension
axis				
comment	NC_CHAR			"X"
long_name	NC_CHAR			"This coordinate variable defines the indices across track, from west to east; index starts at 0"
units	NC_CHAR			"across-track dimension index"
				"1"
scanline				
NC_INT	{# scan lines}			Along-track pixel index dimension
axis				
comment	NC_CHAR			"Y"
	NC_CHAR			"This coordinate variable defines the indices along track; index starts at 0"

long_name	NC_CHAR	“along-track dimension index”	
units	NC_CHAR	“1”	
time			
NC_INT	(1)		Reference time dimension
axis	NC_CHAR	“T”	
comment	NC_CHAR	“The time in this variable corresponds to the time in the time_reference global attribute”	
long_name	NC_CHAR	“reference time for the measurements”	
standard_name	NC_CHAR	“time”	
units	NC_CHAR	“seconds since 2010-01-01 00:00:00”	

The SUPPORT_DATA group

This is a subgroup of PRODUCT. It has its own sub groups and contains no other elements than those.

The DETAILED_RESULTS group

Full path to this group: /PRODUCT/SUPPORT_DATA/DETAILED_RESULTS.

In addition to the main output from the TCBRO processor (the BrO total vertical column density), additional parameters are retrieved along with or are available for diagnostic or statistical purposes. Those are stored in the DETAILED_RESULTS group. The group contains one sub group: WAVELENGTH_CALIBRATION, where all diagnostic parameters regarding the wavelength calibration procedure are stored.

Variables in the group DETAILED_RESULTS:

Name	Type	Size	Unit	Description
Attribute name	Attribute type	Attribute value		
brominemonoxide_geometric_air_mass_factor				
NC_FLOAT	(time, ground_pixel)	scanline,		
coordinates	NC_CHAR	“/PRODUCT/longitude /PRODUCT/latitude”		
long_name	NC_CHAR	“geometric mass factor”		
units	NC_CHAR	“1”		
brominemonoxide_slant_column_corrected				
NC_FLOAT	(time, ground_pixel)	scanline,	mole m ⁻²	The BrO slant column after offset correction.
coordinates	NC_CHAR	“/PRODUCT/longitude /PRODUCT/latitude”		

long_name	NC_CHAR	"corrected slant column density"	
multiplication_factor_to_c onvert_to_DU	NC_FLOAT	2241.15	
multiplication_factor_to_c onvert_to_percm2	NC_FLOAT	6.02214E19	
units	NC_CHAR	"mol m-2"	
brominemonoxide_slant_column_corrected_trueness			
NC_FLOAT	(time, scanline, ground_pixel)	mole m ⁻²	The systematic error un the corrected BrO slant column.
coordinates	NC_CHAR	"/PRODUCT/longitude /PRODUCT/latitude"	
long_name	NC_CHAR	"systematic error of the slant column density"	
multiplication_factor_to_c onvert_to_DU	NC_FLOAT	2241.15	
multiplication_factor_to_c onvert_to_percm2	NC_FLOAT	6.02214E19	
units	NC_CHAR	"mol m-2"	
brominemonoxide_slant_column_correction_flag			
NC_FLOAT	(time, scanline, ground_pixel)	1	
coordinates	NC_CHAR	"/PRODUCT/longitude /PRODUCT/latitude"	
flag_meanings	NC_CHAR	"not-corrected, corrected"	
flag_values	NC_UBYTE	[0,1]	
long_name	NC_CHAR	"slant column density background correction flag"	
units	NC_CHAR	"1"	
brominemonoxide_total_vertical_column_correction			
NC_FLOAT	(time, scanline, ground_pixel)	mole m ⁻²	Correction value on the BrO vertical column.
coordinates	NC_CHAR	"/PRODUCT/longitude /PRODUCT/latitude"	
long_name	NC_CHAR	"background correction value which is added to the vertical column density"	
multiplication_factor_to_c onvert_to_DU	NC_FLOAT	2241.15	
multiplication_factor_to_c onvert_to_percm2	NC_FLOAT	6.02214E19	
units	NC_CHAR	"mol m-2"	
brominemonoxide_total_vertical_column_trueness			

NC_FLOAT	(time, scanline, ground_pixel)	mole m ⁻²	The systematic error un the BrO vertical column.
coordinates	NC_CHAR	"/PRODUCT/longitude /PRODUCT/latitude"	
long_name	NC_CHAR	"systematic error of vertical column density"	
multiplication_factor_to_convert_to_DU	NC_FLOAT	2241.15	
multiplication_factor_to_convert_to_percm2	NC_FLOAT	6.02214E19	
units	NC_CHAR	"mol m-2"	
fitted_radiance_shift			
NC_FLOAT	(time, scanline, ground_pixel)	1	
coordinates	NC_CHAR	"/PRODUCT/longitude /PRODUCT/latitude"	
long_name	NC_CHAR	"radiance wavelength shift from the doas fit"	
units	NC_CHAR	"1"	
fitted_radiance_squeeze			
NC_FLOAT	(time, scanline, ground_pixel)	1	
coordinates	NC_CHAR	"/PRODUCT/longitude /PRODUCT/latitude"	
long_name	NC_CHAR	"radiance wavelength squeeze/stretch from the doas fit"	
units	NC_CHAR	"1"	
fitted_root_mean_square			
NC_FLOAT	(time, scanline, ground_pixel)	1	
coordinates	NC_CHAR	"/PRODUCT/longitude /PRODUCT/latitude"	
long_name	NC_CHAR	"root mean square from the doas fit"	
units	NC_CHAR	"1"	
fitted_slant_columns			
NC_FLOAT	(time, scanline, ground_pixel, number_of_slant_columns)	mol m-2	The retrieved slant column values for all absorbing species.
coordinates	NC_CHAR	"/PRODUCT/longitude /PRODUCT/latitude"	
index_meaning	NC_CHAR	{list of static absorption cross-section input files}	
long_name	NC_CHAR	"slant columns of all absorbers"	
multiplication_factor_to_convert_to_DU	NC_FLOAT	2241.15	

multiplication_factor_to_convert_to_percm2 units	NC_FLOAT NC_CHAR	6.02214E19 "mol m-2"	
fitted_slant_columns_precision			
NC_FLOAT	(time, scanline, ground_pixel, number_of_slant_columns)	mol m-2	Random error on the retrieved slant column values for all absorbing species.
coordinates	NC_CHAR	"/PRODUCT/longitude /PRODUCT/latitude"	
index_meaning	NC_CHAR	{list of static absorption cross-section input files}	
long_name	NC_CHAR	"slant columns errors of all absorbers"	
multiplication_factor_to_convert_to_DU	NC_FLOAT	2241.15	
multiplication_factor_to_convert_to_percm2	NC_FLOAT	6.02214E19	
long_name	NC_CHAR		
units	NC_CHAR	"mol m-2"	
number_of_slant_columns			
NC_INT	(8)		Dimension variable containing the retrieved slant column indices.
long_name	NC_CHAR	"number_of_slant_columns dimension index"	
units	NC_CHAR	"1"	
number_of_spectral_points_in_retrieval			
NC_INT	(time, scanline, ground_pixel)	1	Number of spectral points used in the DOAS retrieval
coordinates	NC_CHAR	"/PRODUCT/longitude /PRODUCT/latitude"	
long_name	NC_CHAR	"Number of spectral points used in the DOAS retrieval"	
units	NC_CHAR	"1"	

Variables in the group DETAILED_RESULTS/WAVELENGTH_CALIBRATION:

Name					
Type	Size	Unit	Description		
Attribute name	Attribute type	Attribute value			
calibration_polynomial_coefficients					
NC_FLOAT	(ground_pixel, degrees_of_polynomial_s hift)	1	Computed coefficients of the DOAS polynomial function.		
long_name	NC_CHAR	"computed coefficients of the polynomial function"			
units	NC_CHAR	"1"			
calibration_subwindows_root_mean_square					
NC_FLOAT	(ground_pixel, number_of_subwindows)	1			
long_name	NC_CHAR	"calibration rms per subwindow"			
units	NC_CHAR	"1"			
calibration_subwindows_shift					
NC_FLOAT	(ground_pixel, number_of_subwindowsl)	1			
long_name	NC_CHAR	"irradiance wavelengths shift fitted values per subwindow"			
units	NC_CHAR	"1"			
calibration_subwindows_squeeze					
NC_FLOAT	(ground_pixel, number_of_subwindows)	1			
long_name	NC_CHAR	"irradiance wavelengths squeeze fitted values per subwindow"			
units	NC_CHAR	"1"			
calibration_subwindows_wavelength					
NC_FLOAT	(number_of_subwindows)	nm			
long_name	NC_CHAR	"calibration wavelength center in each subwindow"			
units	NC_CHAR	"nm"			
degrees_of_polynomial_shift					
NC_INT	(degrees_of_poly nomial_shift)	1	Dimension with polynomial degree indices.		
long_name	NC_CHAR	"degrees_of_polynomial_shift dimension index"			

units	NC_CHAR	"1"	
number_of_calibrations			
NC_INT	(ground_pixel)	1	Dimension array with number of calibration indices (one per detector row).
long_name		"number_of_calibrations dimension index"	
units		"1"	
number_of_subwindows			
NC_INT	{# sub-windows}		Dimension variable containing the sub-window indices.
long_name	NC_CHAR	"number_of_subwindows dimension index"	
units	NC_CHAR	"1"	

The GEOLOCATIONS group

The full path to this group is /PRODUCT/SUPPORT_DATA/GEOLOCATIONS/.

Variable			
Type	Dimensions	Unit	Description
Attribute name	Attribute type	Attribute value	
geolocation_flags			
NC_UBYTE	(time, scanline, ground_pixel)	1	Ground pixel quality flag
coordinates	NC_CHAR	/PRODUCT/longitude /PRODUCT/latitude	
flag_masks	NC_UBYTE	0, 1, 2, 4, 8, 16, 128	
flag_meanings	NC_CHAR	no_error solar_eclipse sun_glint_possible descending night geo_boundary_crossing geolocation_error	
flag_values	NC_UBYTE	0, 1, 2, 4, 8, 16, 128	
long_name	NC_CHAR	"ground pixel quality flag"	
max_val	NC_UBYTE	128	
min_val	NC_UBYTE	0	
units	NC_CHAR	"1"	
latitude_bounds			
NC_FLOAT	(time, scanline, ground_pixel, 4)	degree	Ground pixel corner coordinate latitudes

units	NC_CHAR	“degree north”	
longitude_bounds			
NC_DOUBLE	(time, scanline, ground_pixel, 4)	degree	Ground pixel corner coordinate longitudes
units	NC_CHAR	“degree east”	
satellite_altitude			
NC_FLOAT	(time, scanline)	degree	Satellite altitude
comment	NC_CHAR	“The altitude of the satellite with respect to the geodetic sub satellite point on the WGS84 reference ellipsoid”	
long_name	NC_CHAR	“satellite altitude”	
units	NC_CHAR	“m”	
valid_max	NC_FLOAT	90000.	
valid_min	NC_FLOAT	70000.	
satellite_latitude			
NC_FLOAT	(time, scanline)	degree	Satellite latitude
comment	NC_CHAR	“Latitude of the geodetic sub satellite point on the WGS84 reference ellipsoid”	
long_name	NC_CHAR	“Sub satellite latitude”	
units	NC_CHAR	“degree north”	
valid_max	NC_FLOAT	90.	
valid_min	NC_FLOAT	-90.	
satellite_longitude			
NC_FLOAT	(time, scanline)	degree	Satellite longitude
comment	NC_CHAR	“Longitude of the geodetic sub satellite point on the WGS84 reference ellipsoid”	
long_name	NC_CHAR	“Sub satellite longitude”	
units	NC_CHAR	“degree east”	
valid_max	NC_FLOAT	90.	
valid_min	NC_FLOAT	-90.	
satellite_orbit_phase			
NC_FLOAT	(time, scanline)	1	Satellite fractional orbit phase
comment	NC_CHAR	“Relative offset [0.0, ..., 1.0] of the measurement in the orbit”	
long_name	NC_CHAR	“fractional satellite orbit phase”	
units	NC_CHAR	“1”	

valid_max	NC_FLOAT	1.02	
valid_min	NC_FLOAT	-1.02	
solar_azimuth_angle			
NC_DOUBLE	(time, scanline, ground_pixel)	degree	Solar azimuth angle
comments	NC_CHAR	"Solar azimuth angle at the ground pixel location on the reference ellipsoid. Angle is measured clockwise from the North (East = 90, South = 180, West = -180)"	
coordinates	NC_CHAR	"/PRODUCT/longitude /PRODUCT/latitude"	
long_name	NC_CHAR	"solar azimuth angle"	
standard_name	NC_CHAR	"solar_azimuth_angle"	
units	NC_CHAR	"1"	
valid_max	NC_FLOAT	180.	
valid_min	NC_FLOAT	-180.	
solar zenith angle			
NC_DOUBLE	(time, scanline, ground_pixel)	degree	Solar zenith angle
comments	NC_CHAR	"Solar zenith angle at the ground pixel location on the reference ellipsoid. Angle is measured away from the vertical"	
coordinates	NC_CHAR	"/PRODUCT/longitude /PRODUCT/latitude"	
long_name	NC_CHAR	"solar zenith angle"	
standard_name	NC_CHAR	"solar_z zenith_angle"	
units	NC_CHAR	"1"	
valid_max	NC_FLOAT	180.	
valid_min	NC_FLOAT	0.	
viewing_azimuth_angle			
NC_DOUBLE	(Time, scanline, ground_pixel)	degree	Viewing azimuth angle
comments	NC_CHAR	"Satellite azimuth angle at the ground pixel location on the reference ellipsoid. Angle is measured clockwise from the North (East = 90, South = 180, West = -180)"	
coordinates	NC_CHAR	"/PRODUCT/longitude /PRODUCT/latitude"	
long_name	NC_CHAR	"viewing azimuth angle"	
standard_name	NC_CHAR	"viewing_azimuth_angle"	
units	NC_CHAR	"1"	
valid_max	NC_FLOAT	180.	
valid_min	NC_FLOAT	-180.	

viewing_zenith_angle			
NC_DOUBLE	(Time, scanline, ground_pixel)	degree	Viewing zenith angle
comments	NC_CHAR	"Zenith angle of the satellite at the ground pixel location on the reference ellipsoid. Angle is measured away from the vertical"	
coordinates	NC_CHAR	"/PRODUCT/longitude /PRODUCT/latitude"	
long_name	NC_CHAR	"viewing zenith angle"	
standard_name	NC_CHAR	"viewing_zenith_angle"	
units	NC_CHAR	"1"	
valid_max	NC_FLOAT	180.	
valid_min	NC_FLOAT	0.	

The INPUT_DATA group

This group contains the parameters that serve as input to the TCBRO processor. This group also contains one sub group: BACKGROUND_CORRECTION, that contains all quantities that are required for the slant column background correction procedure.

Variables in INPUT_DATA

Variable			
Type	Dimensions	Unit	Description
Attribute name	Attribute type	Attribute value	
instrument_configuration_identifier			
NC_INT	(time, scanline)	1	Each combination of instrument settings is referred to as an instrument configuration and is identified by an instrument configuration ID, a number in the range [1;65535].
comment	NC_CHAR	"The Instrument Configuration ID defines the type of measurement and its purpose. The number of instrument configuration IDs will increase over the mission as new types of measurements are created and used"	
long_name	NC_CHAR	"IcID"	

The INPUT_DATA/BACKGROUND_CORRECTION group

Attribute	Attribute type	Attribute value	Description
reference_radiance_time_range	NC_CHAR	{"YYYYMMDDThhmmss_YYYYMMDDThhmmss "}	Time interval (start_end) of the measurements used to determine the radiance reference spectra.
background_scd_time_range	NC_CHAR	{"YYYYMMDDThhmmss_YYYYMMDDThhmmss "}	Time interval (start_end) of the measurements used to derive the slant column values over the reference region..

Variables in INPUT_DATA/BACKGROUND_CORRECTION

Variable	Type	Dimensions	Unit	Description
Attribute name	Attribute type	Attribute value		
amf_scd0_average				
NC_FLOAT	(ground_pixel)	1		Per-row average geometric amf over the reference sector.
units	NC_CHAR	"1"		
earthshine_reference_radiance				
NC_FLOAT	(ground_pixel, wavelengths)			Radiance reference spectrum per detector row.
units	NC_CHAR	"mol.m-2.nm-1.sr-1.s-1"		
earthshine_reference_wavelength				
NC_FLOAT	(ground_pixel, wavelengths)	nanometer		Radiance reference wavelength grid.
units	NC_CHAR	"nm"		
offsets				
NC_FLOAT	(ground_pixel)	mole m ⁻²	VCD offset .	
units	NC_CHAR	"mol m-2"		
offsets_scd0				
NC_FLOAT	(ground_pixel)	mole m ⁻²	SCD offset.	
units	NC_CHAR	"mol m-2"		

wavelengths			
NC_INT	{# wavelengths}	nanometer	Wavelength dimension index of the reference spectrum.