



EUMETSAT
AC SAF
ATMOSPHERIC COMPOSITION
MONITORING

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EUMETSAT

AC SAF

ATMOSPHERIC COMPOSITION
MONITORING

PRODUCT USER MANUAL

GOME-2 tropospheric BrO data-records

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TABLE OF CONTENTS

EUMETSAT Satellite Application Facility on Atmospheric Composition Monitoring (AC SAF)	5
Background.....	5
Objective.....	5
Product categories, timeliness and dissemination	5
More information about the AC SAF project, products and services:	6
AC SAF Helpdesk	6
1. Introduction	7
1.1 Purpose and Scope	7
1.2 References	8
1.2.1 Applicable Documents	8
1.2.2 Reference Documents	8
1.3 Abbreviations and Acronyms	9
2. GOME Instruments	10
2.1 Introduction.....	10
2.2 GOME-2/Metop.....	11
2.3 Measurement Scenarios, Timelines and Instrument Modes	11
3. Algorithm Description	12
3.1 Summary	12
3.2 BrO product	12
3.3 GOME-2/Metop processing chain	12
3.4 Data Management	13
3.5 Quality Control and Monitoring.....	14
3.6 Geophysical Validation	14
3.7 User Services	14
4. Column Trace Gases and Cloud Products	16
4.1 Units	16
4.2 Geographical Coverage and Granularity	16
4.3 Spatial Resolution.....	16
4.4 Delivery Time.....	16
4.5 Expected Accuracy	17
4.6 Product Formats	17
4.7 File Name	17
4.8 Product Dissemination	17
4.9 Product Ordering	18

5.	NetCDF4 Product Format Description	19
5.1	META_DATA Group	20
5.2	PRODUCT Group	24
5.3	DETAILED_RESULTS Group	25
5.4	GEOLOCATION Group.....	27
5.5	INPUT_DATA Group.....	28
5.6	Detailed Flag Description	29
5.6.1	SwathMode and ViewMode	29
5.6.2	surface_condition flags	29
5.6.3	snow_ice_flag	30
5.6.4	processing_quality_flag	30
5.6.5	Flag usage.....	30
6.	Using the Products.....	32
6.1	Confidence Flags and Ancillary Fields	32
6.2	Averaging Kernels	32
6.3	Software and Tools for reading the products.....	33

EUMETSAT SATELLITE APPLICATION FACILITY ON ATMOSPHERIC COMPOSITION MONITORING (AC SAF)

Background

The need for atmospheric chemistry monitoring was first realized when severe loss of stratospheric ozone was detected over the Polar Regions. At the same time, increased levels of ultraviolet radiation were observed.

Ultraviolet radiation is known to be dangerous to humans and animals (causing e.g. skin cancer, cataract, immune suppression) and having harmful effects on agriculture, forests and oceanic food chain. In addition, the global warming - besides affecting the atmospheric chemistry - also enhances the ozone depletion by cooling the stratosphere. Combined, these phenomena have immense effects on the whole planet. Therefore, monitoring the chemical composition of the atmosphere is a very important duty for EUMETSAT and the world-wide scientific community.

Objective

The main objectives of the AC SAF are to process, archive, validate and disseminate atmospheric composition products (O_3 , NO_2 , SO_2 , BrO, HCHO, H_2O and OCIO), aerosol products and surface ultraviolet radiation products utilising the satellites of EUMETSAT. The majority of the AC SAF products are based on data from the GOME-2 spectrometers onboard Metop-A, Metop-B and Metop-C satellites.

Another important task of the AC SAF is the research and development in radiative transfer modelling and inversion methods for obtaining long-term, high-quality atmospheric composition products from the satellite measurements.

Product categories, timeliness and dissemination

Data products are divided in two categories depending on how quickly they are available to users:

Near real-time products are available in less than three hours after measurement. These products are disseminated via EUMETCast, WMO GTS or internet.

- Near real-time trace gas columns
 O_3 , NO_2 , HCHO, SO_2
- Near real-time ozone profiles
coarse and high-resolution
- Near real-time absorbing aerosol indexes
from main science channels and polarization measurement detectors
- Near real-time UV indexes
clear-sky and cloud-corrected

Offline products are available in two weeks after measurement and disseminated via dedicated web services at EUMETSAT, FMI and DLR.

- Offline trace gas columns
 O_3 , NO_2 , SO_2 , BrO, HCHO, H_2O and OCIO
- Offline ozone profiles
coarse and high-resolution
- Offline absorbing aerosol indexes

from main science channels and polarization measurement detectors

- Offline surface UV

Data records products are available for a fixed time range, e.g. 23.1.2007 to 27.6.2020 for tropospheric BrO. In contrast to the NRTI and OFFL data the datasets are not automatically continued based on new observations. The respective data sets are disseminated via dedicated web services at EUMETSAT, FMI and DLR. Available datasets are:

- Tropospheric BrO columns
- Glyoxal columns
- Monthly gridded tropospheric NO₂ and H₂O columns

More information about the AC SAF project, products and services:

<http://acsaf.org/>

AC SAF Helpdesk: helpdesk@acsaf.org

1. INTRODUCTION

1.1 Purpose and Scope

DLR produces on an operational basis a range of total column trace gases and cloud products for the GOME-2 instruments on Metop-A, -B and -C in the framework of EUMETSAT's AC SAF.

DLR has a long experience in operational processing of GOME-2 data. This document is the user manual for the GOME-2/Metop -A and -B tropospheric Bromine monoxide data records available at DLR.

DLR provides near-real-time (NRT), off-line (OL), and reprocessed products and data-records. The NRT products have the same granularity as the input GOME-2 data (i.e. downlink or PDU) and are made available and disseminated to the users within 2 hours 30 minutes of sensing. The OL products are consolidated orbits from ascending node crossing to ascending node crossing and are available and disseminated to the users within two weeks after sensing.

Additionally, DLR provides reprocessed products and data records for the complete GOME-2/Metop-A data record starting in Jan. 2007, and the GOME-2/Metop-B data record starting in Jan. 2013.

The network Common Data Format (netCDF version4) has been selected as data format for the GOME-2 tropospheric BrO data records. NetCDF is a self-describing, machine-independent file formats commonly used for storage and transfer of scientific and meteorological data, it is based on the HDF5 (Hierarchical Data Format) which is also used frequently (including AC-SAF total common results)

The present document is divided into the following sections:

- Overview of the GOME-2 instruments on Metop-A, -B and -C including instrument modes
- Summary of the algorithm used for the retrieval of tropospheric BrO columns
- Summary of the processing chain
- Product description including the used netCDF4 format

1.2 References

1.2.1 Applicable Documents

- [A1] [A1] AC SAF Product Requirements Document, Issue 1.5, SAF/AC/FMI/RQ/PRD/001, Hovila et al., 2019.

1.2.2 Reference Documents

- [R1] Algorithm Theoretical Basis Document for GOME-2 Total Column Products of Ozone, NO₂, BrO, SO₂, H₂O, HCHO, OCIO and Cloud Properties (GDP 4.8/4.9), SAF/AC/DLR/ATBD/01, Iss. 3/B, Valks, P., et al., 2019.
- [R2] Algorithm Theoretical Basis Document for GOME-2 tropospheric Bromine Monoxide columns, SAF/AC/DLR/ATBD/BrOTrop/01, Iss. 1/B, Heue et al., 2020
- [R3] GOME-2 Level 1 Product Format Specification, EPS/MIS/SPE/97232, v9D, March 2012.
- [R4] GOME-2 Level 2 Product User Manual (PUM) of Total Column Products of Ozone, NO₂, BrO, HCHO, SO₂, H₂O, OCIO and Cloud Properties (GDP 4.8/4.9) SAF/AC/DLR/PUM/01, Iss. 3/B Valks, P., et al., Nov. 2019
- [R5] Algorithm Theoretical Basis Document for GOME-2 surface LER product, SAF/AC/KNMI/ATBD/003, Iss 3.1, Tilstra et al. March 2019.
- [R6] GOME-2 GDP 4.8 BrO tropospheric column validation report, SAF/O3M/BIRA/VR/BRO, Theys et al., November 2020.
- [R7] NetCDF4 Format description <https://www.unidata.ucar.edu/software/netcdf/>
- [R8] Eumetcast Dissemination Facility
<http://www.eumetsat.int/website/home/Data/DataDelivery/EUMETCast/index.html>
- [R9] Eoweb DLR Online User Service <http://eoweb.dlr.de>
- [R10] Global Sea Ice Concentration Climate DataRecordProduct User ManualProduct OSI-450 & OSI-430-bDocument version: 2.0 Data set version: 2.0
DOI: 10.15770/EUM_SAF_OSI_0008 March 2019
http://osisaf.met.no/docs/osisaf_cdop3_ss2_pum_sea-ice-conc-climate-data-record_v2p0.pdf

1.3 Abbreviations and Acronyms

A list of abbreviations and acronyms used throughout this document is given below:

AC SAF	SAF on Atmospheric Chemistry Monitoring
AMF	Air Mass Factor
BIRA-IASB	Belgian Institute for Space Aeronomy
CCSDS	Consultative Committee for Space Data Systems
DLR	Deutsches Zentrum für Luft- und Raumfahrt e.V. (German Aerospace Centre)
DOAS	Differential Optical Absorption Spectroscopy
D-PAF	German processing and archiving facility
DU	Dobson Unit
ERS-2	European Remote Sensing Satellite-2
ESA	European Space Agency
ESC	Effective Slant Column
EUMETSAT	European Organisation for the Exploitation of Meteorological Satellites
GDP	GOME Data Processor
GOME	Global Ozone Monitoring Experiment
HDF	Hierarchical Data Format
IMF	Remote Sensing Technology Institute
Metop	Operational Meteorological Satellite
netCDF	network Common Data Format
NRT	Near-Real-Time
NT	Nominal-Time
OL	Off-Line
OTO	Identifier used for off-line total column and cloud products
PDU	Product Dissemination Unit
PMD	Polarisation Measurement Device
RP	Postfix identifier user for reprocessed total column and cloud products
RMS	Root Mean Square
SAF	Satellite Application Facility
SCD	Slant Column Density
SZA	Solar Zenith Angle
TBD	To be Defined
TOA	Top of Atmosphere
UMARF	Unified Meteorological Archiving and Retrieval Facility
UV	Ultra Violet
UTC	Universal Time Coordinate
VCD	Vertical Column Density
VIS	Visible

2. GOME INSTRUMENTS

2.1 Introduction

The Global Ozone Monitoring Experiment (GOME) and GOME-2 instruments are scanning spectrometers that capture light reflected from the Earth's surface and atmosphere. The spectrometer splits the light into its spectral components covering the UV/VIS region from 240 nm to 790 nm at a resolution of 0.2 nm to 0.5 nm.

The measured spectra are mainly used to derive ozone total column and vertical profile, nitrogen dioxide, formaldehyde, bromine oxide, water vapour, sulphur dioxide and other trace gases, as well as cloud properties and aerosols.

The next figure shows a schematic representation of GOME-2 optical layout. A scan mirror directs the light emitted from the Earth's atmosphere or the Sun diffuser into the instrument. The spectrometer splits incoming light into four channels using a complex array of telescopes, prisms and gratings. Detectors at the end of each optical path collect information about the signal in each channel.



Figure 1: GOME-2 optical layout (courtesy of ESA)

2.2 GOME-2/Metop

On 30 January 1998, the ESA Earth Observation Program Board gave its final go-ahead for the Metop Program. The instruments on the Metop satellites are designed to produce high-resolution images of the Earth's surface, vertical temperature and humidity profiles, and temperatures of the land and ocean surface on a global basis. In addition, there are instruments for monitoring trace gases and wind flow over the oceans. This instrument payload is of significant value to meteorologists and other scientists, particularly to those studying the global climate.

Given the need for global-scale routine monitoring of the abundance and distribution of ozone and associated trace gas species, a proposal was put forward for the inclusion of GOME-2 on the Metop satellites. Metop-A was launched on 19 October 2006 as part of the Initial Joint Polar System (IJPS) in co-operation with NOAA in the USA. A second polar-orbiting meteorological satellite in the series, Metop-B, was successfully launched on 17 September 2012. The third and last polar-orbiting satellite in the series, Metop-C, was successfully launched on 7 November 2018.

The GOME-2/Metop field of view of each step may be varied in size from 5 km x 40 km to 80 km x 40 km. The mode with the largest footprint (twenty four steps with a total coverage of 1920 km x 40 km) provides daily near global coverage at the equator [R3].

Based on the successfully work with the GOME Data Processors, the German Aerospace Centre (DLR) plays a major role in the design, implementation and operation of the GOME-2/Metop ground segment for total column products. DLR is a partner in the Satellite Application Facility on Ozone and Atmospheric Chemistry Monitoring (AC-SAF), which is part of the Eumetsat Polar System (EPS) ground segment, and is responsible in this project for the generation of total column amounts of the various trace gases and cloud properties (<https://atmos.eoc.dlr.de/app/missions/gome2>) which may be retrieved from GOME-2/Metop level 1b products.

2.3 Measurement Scenarios, Timelines and Instrument Modes

GOME-2/Metop has several operational scenario, see:

<http://gome.eumetsat.int>

for more details.

- **Earth Observation Mode**
This mode includes nadir/narrow/static/north-polar/south-polar scanning measurements with various integration times depending on solar zenith angle. This is the default mode for the day side. Only the data acquired in this mode are used for geophysical retrievals.
- **Calibration Modes**
This mode includes Sun/Moon/dark/spectral-light/LED/white-light measurements. Most of these calibrations are performed on the night side.

3. ALGORITHM DESCRIPTION

3.1 Summary

The tropospheric bromine monoxide (BrO) retrieval is based on the GOME-2 BrO slant columns retrieved from the Level 1 data [R3]. The retrieval uses a DOAS fit to retrieve slant column densities (SCD) of several trace gases from the measured spectra. The BrO SCD fit is performed in a fitting window between 332 and 359 nm. During a calibration pre fit the GOME-2 slit function is optimized, the cross-sections of NO₂, BrO, OCIO and O₃ (223 and 243K) are convoluted online using the optimised slit function. The DOAS slant column retrieval is followed by the Air Mass Factor (AMF) conversions to generate vertical column densities. Cloud information used in the trace gas retrieval is obtained with the OCRA and ROCINN algorithms. A detailed description of the operational GOME-2 L2 cloud algorithms is given in [R1].

3.2 BrO product

The first step during the extraction of tropospheric BrO is a tropical background correction of the SCDs. The SCDs for one day are averaged between 5° South and 5° North and a mean stratospheric SCD of $7.5 \cdot 10^{13}$ mole/cm² is assumed. The stratospheric slant column is calculated from a BrO/Br_y climatological ratio that among other parameters depends on the stratospheric NO₂ columns and a Br_y climatology which is correlated to the O₃ column. The climatologies were calculated at BIRA using the BRAM assimilation tool. The O₃ and NO₂ column data are read from the operational GOME-2 level 2 data products. For the conversion of the tropospheric slant columns to tropospheric vertical columns a lookup table based on Lidort calculations is used. The SZA of LUT ranges up to 85° thereby the data range is limited to a solar zenith angle less than 85°. However, often the data are masked out due to other limitation (quality flag 5.6.4) already for lower SZA. The tropospheric BrO apriori profile depends on the surface albedo. An elevated Gaussian distribution is assumed for albedo values lower than 0.5 and a box function for the lowest 2 km above the surface is assumed for high albedo cases such as snow or ice.

The albedo data are taken from the AC SAF GOME-2 DLER climatology [R5]. The daily snow cover is updated based on the ECMWF ERA5 reanalysis and sea-ice cover is downloaded from OSI-SAF project (<http://osisaf.met.no/p/ice/>, Copyright 2020 EUMETSAT [R10]) to update the albedo values according to the actual snow and ice cover. The Tropopause level is calculated based on the ECMWF ERA PV and temperature datasets. The 3.5 PVU isoline is used in the polar to mid latitudes and 380K potential temperature in the tropics, additional details are given in [R2].

Table 1: GOME-2 tropospheric BrO column products from Metop-A and –B provided by the AC SAF

Data-record	AC SAF identifier	Wavelength region (nm)	Period for GOME-2A	Period for GOME-2B
Tropospheric BrO columns	O3M-116.0	332.0-359.0	23. Jan 2007 - 31. Dec. 2018	1. Jan 2013- 30. June 2020

3.3 GOME-2/Metop processing chain

DLR has developed the operational processing chain for GOME-2/Metop total column products. The level 1b products are generated at the EPS ground segment in EUMETSAT [R3] and received at DLR via EUMETCast ([R7]). DLR generates GOME-2/Metop level 2 total column and cloud products.

There are different modules for quality control and monitoring, production control, archiving and order handling. The level 2 products generated at DLR are validated on a regular basis by the AC-SAF partner institutes AUTH, BIRA, and FMI. The GOME-2/Metop level 2 NRT products are disseminated primarily with EUMETCast, WMO/GTS and internet. The off-line products are disseminated via Internet and media. The ordering of products can be done via dedicated user services.

The GOME-2/Metop level 1 products are delivered in NRT (approx. 1:45 hours after sensing) in so called PDU files (product dissemination unit) containing 3 minutes of measurements via EUMETCast. The ground-segment at DLR needs less than 15 minutes for acquiring the input data, retrieving the trace gas total columns and disseminating the resulting level 2 products (Figure 2), that means the GOME-2/Metop total column products are available to the users in less than 2 hours after sensing.

The GOME-2/Metop operational processing is performed in a high availability virtualized environment on a blade center farm.

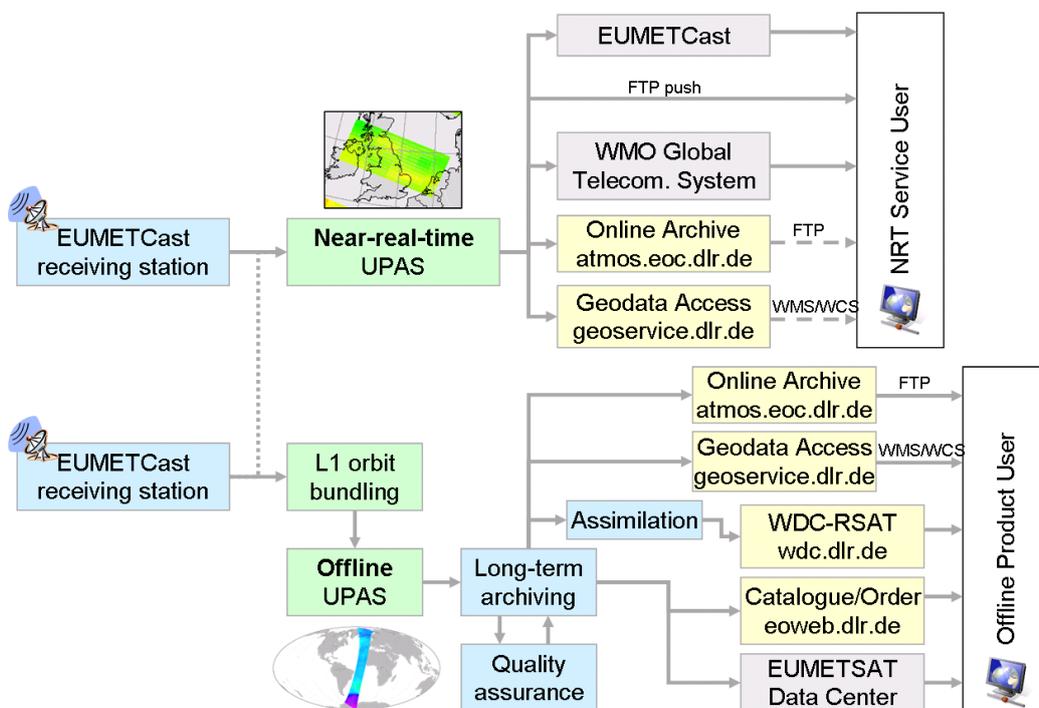


Figure 2: GOME-2/Metop processing chain

3.4 Data Management

The processing of GOME-2/Metop data is embedded in DLR's multi-mission facility ensuring high availability and sustainability. The German National Remote Sensing Data Library stores the data for the long-term enabling monitoring of global change and data reprocessing based on enhanced methodology.

Information and data of AC-SAF products generated at DLR are disseminated through different channels: through direct FTP-push to authorized users and through the EUMETCast broadcast system for near-real-time users, through the EUMETSAT user services.

3.5 Quality Control and Monitoring

The quality of the off-line products is controlled before they are archived and disseminated to the users. A dedicated quality control tool integrated into DLR's data management system displays a set of parameters generated automatically by UPAS for each processed orbit. The quality control tool performs limit checks and computes some statistics to show the confidence levels of the product and its evolution within time.

3.6 Geophysical Validation

The geophysical validation of the official GOME products is performed by an independent partner organization: BIRA. The validation is accomplished using ground-based measurements from the MAX-DOAS networks and other satellite data. The validation results [R5] are publicly available on the Internet, see Section 4.9

3.7 User Services

Information about data and services are accessible through the websites given at the end of this section. The central point of access to this GOME-2 L2 trace gas column data is the AC SAF web-portal at FMI:

<http://acsaf.org>

The data are provided via ftp and can be directly downloaded via: <ftp://acsaf.eoc.dlr.de>

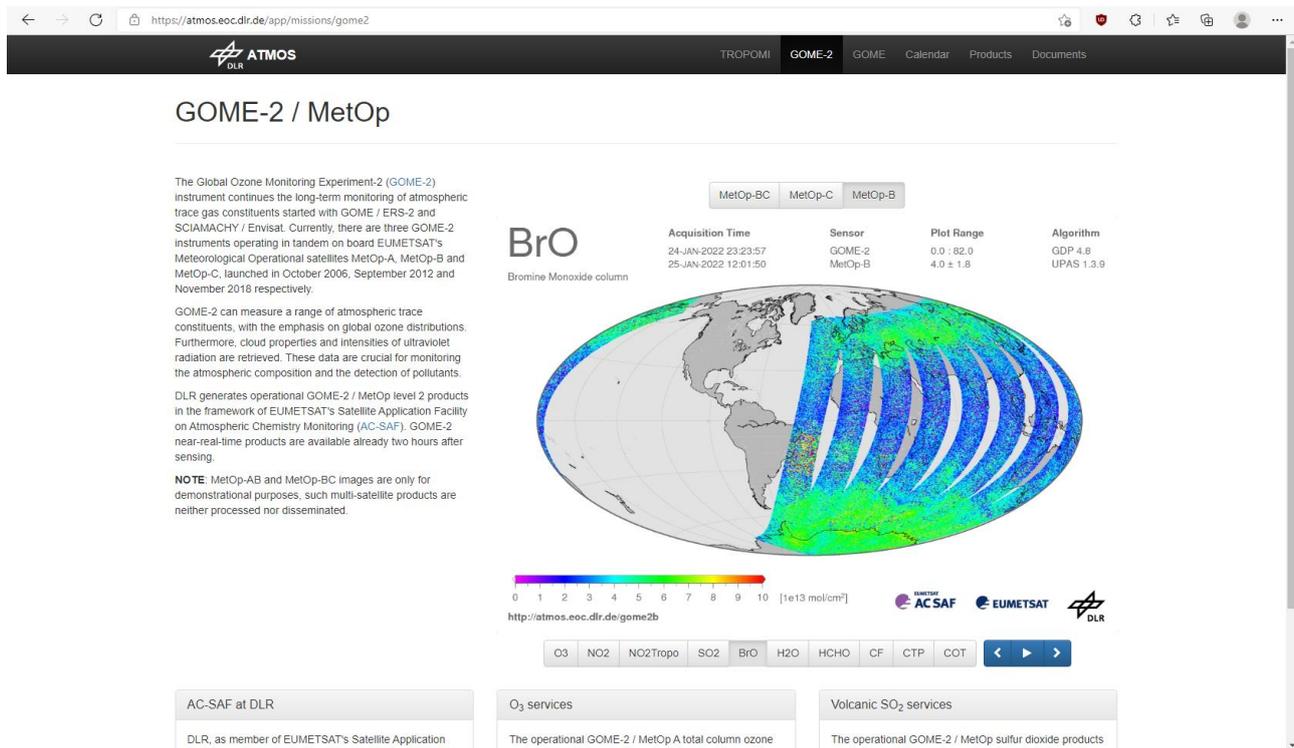


Figure 3: GOME-2 Metop web-page at DLR.

GOME-2A Oper2 BrO tropo VCD (molec/cm²) 2008.03

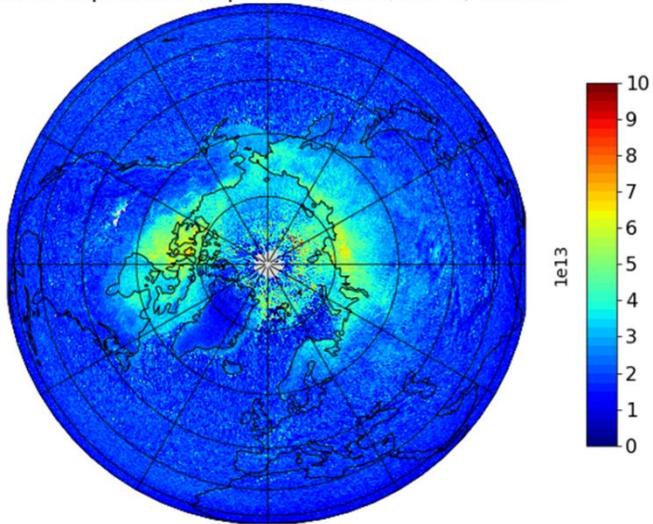


Figure 4: Example results for mean Tropospheric BrO based on GOME-2A observation from March 2008.

4. COLUMN TRACE GASES AND CLOUD PRODUCTS

The GOME-2 level 2 column products contain retrieved trace gas vertical columns and cloud properties, as well as other geophysical parameters; corresponding errors on these quantities, and a number of additional diagnostics, quality flags and intermediate results.

4.1 Units

Table 1: Overview of the units used for the quantities given in the Tropospheric BrO result files.

Dataset	Units
Total ozone column	[DU]
Other trace gas column amounts	[molecules/cm ²]
Cloud fraction and cloud-top albedo (optical thickness)	(unitless) [1]
Height	[km]
Pressure	[hPa]
Angles are given at Top-of-Atmosphere (TOA) (70 km)	[0 to 360 degrees]
Geographical Coordinates	longitude [-180 to +180 degrees] latitude [-90 to +90 degrees]
Errors	absolute values [molecules/cm ²] or [DU]

4.2 Geographical Coverage and Granularity

GOME-2/Metop has a daily near global coverage at the equator. Depending on the scanning mode used, the measured ground pattern may be different.

The NRT, off-line and reprocessed/data-records products have by default a global coverage. The coverage of trace gases available only under special conditions may be reduced.

The NRT products have the same granularity as the downlink or PDU. The off-line and reprocessed products are consolidated orbits from ascending node to ascending node.

4.3 Spatial Resolution

GOME-2/Metop has 24 forward-scan pixels with a nominal resolution of 40 km x 80 km. In the tandem mode, GOME-2/Metop-A operates on a reduced swath width of 960 km with an increased spatial resolution (approx. 40 km x 40 km), while GOME-2/Metop-B and -C operate on a nominal wide swath at 1920 km. This implementation increases both the daily coverage and the spatial resolution of GOME-2 measurements. GOME-2 tandem operations started on 15 July 2013. Only forward scan pixels are processed and written to the tropospheric BrO products.

4.4 Delivery Time

DLR generates near-real-time (NRT), off-line (OL), and reprocessed products (RP). The NRT products are available for distribution in less than 15 minutes after the reception of the GOME-2 level 1 product.

Assuming that the input data is received at DLR 1:45 hours after sensing, then the GOME-2 total column products will be disseminated to the users in less than 2 hours after sensing.

The GOME-2/Metop OL products are available within two weeks after sensing.

Reprocessed GOME-2/Metop level 2 products (data-records) are generated on a regular basis.

4.5 Expected Accuracy

Detailed estimates of the uncertainties in each of the GOME-2 trace gas column products are provided in the ATBD [R1].

4.6 Product Formats

The format of the product file is netCDF4. A detailed description of the product format is given in Chap. 5.

4.7 File Name

The file name of a product already contains important information about the dataset including trace gases and sensing time. It is built according to the following structure:

SENSOR_GAS_LV_YYYYMMDDhhmmss_ddd_MISSION_#####_PRO_RV.TYPE

- SENSOR denotes the instrument, i.e. GOME
- GAS is a "-" separated list of trace gases included in the product i.e. "BrOTropo" is a product containing only bromine monoxide
- LV is the product level, i.e. L2
- YYYYMMDD are the year, month and day of the first processed ground pixel
- hhmmss are the hours, minutes and seconds of the UTC time stamp of the first processed ground pixel
- ddd is the three digit duration of the product in minutes
- MISSION denotes the mission: METOPA, METOPB
- ##### is the five digit orbit number
- PRO is the processing center, i.e. DLR
- RV is the two digit product revision
- TYPE denotes the product format used: netCDF4

The following example is a typical name for a GOME-2/Metop-A product:

GOME_BrOTropo_L2_2007030211155_047_METOPA_01900_DLR_05.nc

4.8 Product Dissemination

The GOME-2/Metop data set products are available at the DLR AC SAF FTP-server (anonymous login):

<ftp://acsaf.eoc.dlr.de/>

The products are organized in directories YYYY/MM/DD where YYYY is the year, MM the month, DD the day.

4.9 Product Ordering

The GOME-2/Metop total column products are generated at DLR in the framework of EUMETSAT's AC SAF



For information and access to all AC SAF products, please refer to the AC SAF web page and help desk:

AC SAF Web page

<http://www.acsaf.org>

AC SAF Helpdesk
helpdesk@acsaf.org

Additional information can be found in EUMETSAT's product Navigator accessible through the following link:

<http://navigator.eumetsat.int/>

Current and historical quick look images of other trace gas products as well as value added products generated by DLR are available at:

<http://atmos.eoc.dlr.de/gome2>

5. NETCDF4 PRODUCT FORMAT DESCRIPTION

The NetCDF4 file structure of the GOME-2 BrOTropo column data is explained below. The DATA GROUPS are written in CAPITAL letters, the variables are written in small letters. All variables are stored in a 2D format (groundpixel x scanlines). Groundpixel 0 is in the east and groundpixel 23 in the western part of the scanline. All data are geo-referenced.

On the top level the file is divided in META_DATA and PRODUCT groups. The META_DATA contains relevant metadata, like orbit number or start time.

The PRODUCT group contains the main results bromine monoxide tropospheric column, as well as latitude and longitude of the pixels centre coordinates and the subgroup SUPPORT_DATA. In the subgroup additional information is provided depending on whether it is part of the analysis process e.g. DOAS results or position data e.g. viewing geometry or additional information that is provided by external sources e.g. surface albedo the data are stored in the DETAILED_RESULTS, GEOLOCATION, or INPUT_DATA respectively.

The product content comprises the following groups:

- META_DATA
 - AC_SAF_METADATA
see section 5.1
- PRODUCT
see section 5.2
 - SUPPORT_DATA
 - DETAILED_RESULTS
see section 5.3
 - GEOLOCATIONS
see section 5.4
 - INPUT_DATA
see section 5.5

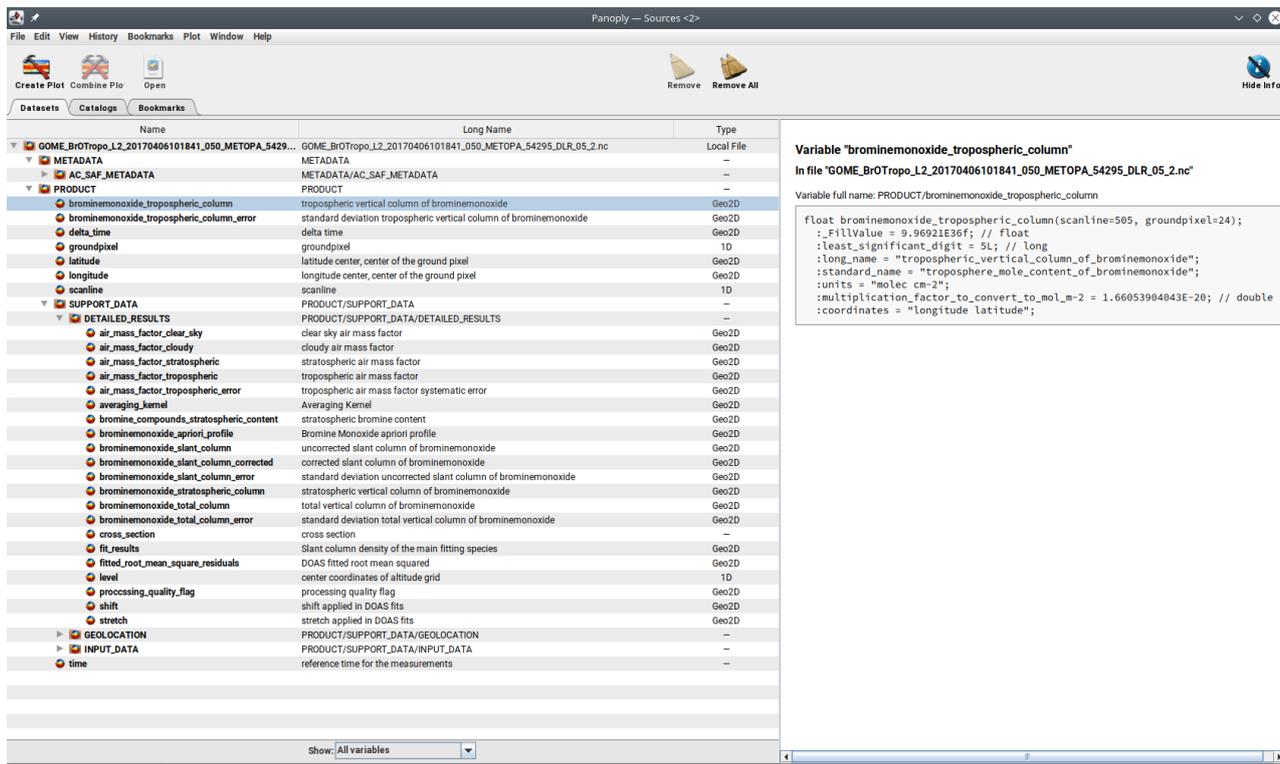


Figure 5: Screenshot of a tropospheric BrO file opened with Panoply

5.1 META_DATA Group

The content of the META_DATA group is shown in the following table. Allowed values specified in italics indicate any value of the given type.

Attribute Name	Data Type	Description	Allowed Values
ArchiveFacility	string	Centre where the data is archived.	O3DLR
SatelliteID	string	Platform identifier and spacecraft).	Mnn
Satellites	string	Platform name	Metop
StartOrbitNumber	integer	Orbit number at the start of sensing, i.e. at the beginning of a dump.	integer
InstrumentID	string	Instrument which acquired the product	GOME_2

Attribute Name	Data Type	Description	Allowed Values
InstrumentMode	VIEW_MODES structure	Specifies how many ground pixels were observed in the corresponding view modes.	VIEW_MODES structure
SensingStartTime	CCSDS_ASCII	UTC date and time at sensing start.	Date in CCSDS format (ASCII)
SensingEndTime	CCSDS_ASCII	UTC date and time at sensing end.	Date in CCSDS format (ASCII)
ReceivingCentre	string	Centre that received the data.	ECF (for EECF), FBK, FUC, GCA, PGS, RUS, SOC, SVL, UBI, WAL, WEC, WIV
ProcessingCentre	string	Centre that generated the data.	O3DLR
ProcessingMode	string	Processing mode applied for generation of the product.	N (nominal), B (backlogged), R (reprocessed), V (validation) T (near-real-time)
Revision	string	Global product revision, required e.g. for reprocessing, part of logical product identifier.	string
ProductType	string	Description of the product type	AC BrOTropo
ProductID	string	AC SAF identifier	O3M-116
ProcessingLevel	string	Processing level applied for generation of the product.	02
ProcessingTime	CCSDS_ASCII	UTC date and time at processing finish.	CCSDS Date
BaseProductAlgorithmVersion	string	Version of the algorithm used to generate the L1B parent product upon which the L2 product is based.	string

Attribute Name	Data Type	Description	Allowed Values
BaseProductsName	string	Name of the Level1 spectra file	string
L2BaseProductName	string	Name of the Level2 data file for clouds, O3 and NO2	string
IceCoverNames	string	Name of the Ice cover data file	string
FileName	string	Name of the Tropospheric BrO data file	string
ProductAlgorithmName	string	Version of the algorithm that produced the product.	G2_L2_BrOTropo
ProductAlgorithmVersion	string	Version of the algorithm that produced the product.	float (two digits)
InternalProcessorRevision	string	Version of the processor used to generate this product.	float (two digits)
ProductFormatType	string	Data format of the product.	netCDF
ProductFormatVersion	string	Version number of the product format.	4
Conventions	string	Climate and Forecast convention for variable names, units and dates	CF-x.y
ProductContents	string	Trace gase included in the product	BrOTropo
SolarSpectraDate	CCSDS_ASCII, string	Date and time of the DOAS reference spectra	CCSDS Date, earthshine
NumberGroundPixels	integer	Number of ground pixels per scanline	int (24)
NumberScanlines	integer	Number of scanlines in the file	int
NumberOfTotalPixels	integer	NumberGroundPixel x NumberScanlines	
MissingDataCount	integer	Number of missing data records.	int

Attribute Name	Data Type	Description	Allowed Values
MissingDataPercentage	integer	Percentage of missing data records.	0-100%
SubsettingRegion	string	Description of the sub setting region. "full" means: no subsisting was applied.	string
SubSatellitePointStartLat	float	Latitude of the sub-satellite point at start of acquisition. (For EPS products: either the first measurement or first complete scan start point (tbd), at start of dataset.)	-90... 90
SubSatellitePointStartLon	float	Longitude of the sub-satellite point at start of acquisition.	0... 360
SubSatellitePointEndLat	float	Latitude of the sub-satellite point at end of acquisition.	-90... 90
SubSatellitePointEndLon	float	Longitude of the sub-satellite point at end of acquisition.	0... 360
SatellitePosition	POS_VEC	Position vectors (X,Y,Z) in km	Vector in POS_VEC
SatelliteVelocity	POS_VEC	Velocity vector (dx/dt, dy/dt, dz/dt) in km/s	Vector in POS_VEC
OrbitSemiMajorAxis	float	Semi-major axis (km)	float
OrbitExcentricity	float	Excentricity	float
OrbitInclination	float	Inclination (deg)	float
OrbitRightAscOfAscNode	float	Right asc. of asc. node (deg)	float
OrbitArgumentOfPerigee	float	Argument of perigee (deg)	float
OrbitMeanAnomaly	float	Orbit mean anomaly (deg)	float
OrbitUTCDaysSince2000	integer	UTC days since 1.1.2000	int

Attribute Name	Data Type	Description	Allowed Values
OrbitMsSinceMidnight	integer	UTC ms since midnight	int
OrbitAscendingNodeCrossingDateTime	CCSDS_ASCII	Ascending node crossing UTC date and time	CCSDS Date
OrbitAscendingNodeLongitude	float	Ascending node longitude	-180... 180
OrbitActualDuration	integer	Orbit duration in minutes, only counting valid pixels	0...~60

5.2 PRODUCT Group

The tropospheric Bromine Monoxide columns are stored in the PRODUCT group together with some essential additional variables. Additional results are given in the respective subgroups of PRODUCT/SUPPORT_DATA. The following table contains the variables in the PRODUCT group.

Dataset Name	Data Type	Dimensions	Unit	Description
brominemonoxide_tropospheric_column	float	scanlines x groundpixel	molecules/cm ²	troposphere_mole_content_of_bromine_monoxide
brominemonoxide_tropospheric_column_error	float	scanlines x groundpixel	molecules/cm ²	troposphere_mole_content_of_bromine_monoxide error
latitude	float	scanlines x groundpixel	° North	latitude of the Pixel Centre (point F in figure 5) (-90° to 90°)
longitude	float	scanlines x groundpixel	° East	longitude of the Pixel Centre (point F in figure 5) (-180° to 180°)
delta_time	float	scanlines x groundpixel	milliseconds	milliseconds since midnight of the reference day reference day is given as attribute
time	integer	1	Seconds	to reference day since midnight 2000-01-01
scanline	integer	Scanlines	1	dimension variable counting the scans from North to South
groundpixel	integer	groundpixel	1	dimension variable counting the groundpixel from East to West

The time format is adapted from the Sentinel 5P operational products. The measurement time is given in the delta_time variable, as milliseconds since midnight of the reference day. The reference day is given in three different variables or attributes. First it is given as attribute to the delta_time variable in the "YYYY-MM-DD" format. It is also given in days since 2000-01-01 in the global file

attributes (OrbitUTCDaysSince2000), or it is given in the time variable in seconds since 2000-01-01. The global attribute and the time variable therefore differ by the constant factor 24×3600 .

5.3 DETAILED_RESULTS Group

The DETAILED_RESULTS group encompasses additional results that are related to the tropospheric bromine monoxide column. The following table gives an overview of all the data in the subgroup.

Dataset Name	Data Type	Dimension	Unit	Description
air_mass_factor_clear_sky	float	scanline x groundpixel	1	clear sky air mass factor
air_mass_factor_cloudy	float	scanline x groundpixel	1	cloudy sky air mass factor
air_mass_factor_stratospheric	float	scanline x groundpixel	1	air mass factor for the stratosphere
air_mass_factor_tropospheric	float	scanline x groundpixel	1	air mass factor for the troposphere
air_mass_factor_tropospheric_error	float	scanline x groundpixel	1	air mass factor for the troposphere error
bromine_compounds_stratospheric_content	float	scanline x groundpixel	molecules/cm3	stratosphere content of bromine species
brominemonoxide_stratospheric_column	float	scanline x groundpixel	molecules/cm2	stratosphere content of bromine monoxide
brominemonoxide_total_column	float	scanline x groundpixel	molecules/cm2	atmosphere content of bromine monoxide
brominemonoxide_total_column_error	float	scanline x groundpixel	molecules/cm2	Atmosphere content of bromine monoxide error
brominemonoxide_slant_column	float	scanline x groundpixel	molecules/cm2	bromine monoxide slant column uncorrected
brominemonoxide_slant_column_corrected	float	scanline x groundpixel	molecules/cm2	bromine monoxide slant column corrected
brominemonoxide_slant_column_error	float	scanline x groundpixel	molecules/cm2	bromine monoxide slant column error
fit_result	float	scanline x groundpixel x cross_sections	molecules/cm2	slant columns of the other absorbers in the DOAS fit
cross_sections	string	cross_sections	--	dimension variable cross section names of the other absorbers O3_228K, O3_243K, O3_XS*λ, O3_XS2, NO2, HCHO, OCIO, Ring_1, Ring_2

Dataset Name	Data Type	Dimension	Unit	Description
fitted_root_mean_square_residuals	float	scanline x groundpixel	1	root mean squared residual of the DOAS fit
level	float	level	km	dimension variable centre of the altitude grid above sea level
shift	float	scanline x groundpixel	nm	shift applied to the wavelength calibration of the spectrum in the DOAS fit
stretch	float	scanline x groundpixel	1	stretch applied to the wavelength calibration of the spectrum in the DOAS fit
averaging_kernel	float	scanline x groundpixel x levels	1	averaging kernel
apriori_profile_bro	float	scanline x groundpixel x levels	molecules/cm ³	apriori profile of BrO for the AMF calculation
processing_quality_flags	integer	scanline x groundpixel	1	quality indicator 0 is good data see section 5.5 flag description

5.4 GEOLOCATION Group

The GEOLOCATION group contains information for the four corner points for the ground pixel, denoted by letters A to D in Figure 6. As well as the viewing geometry for the central point F.

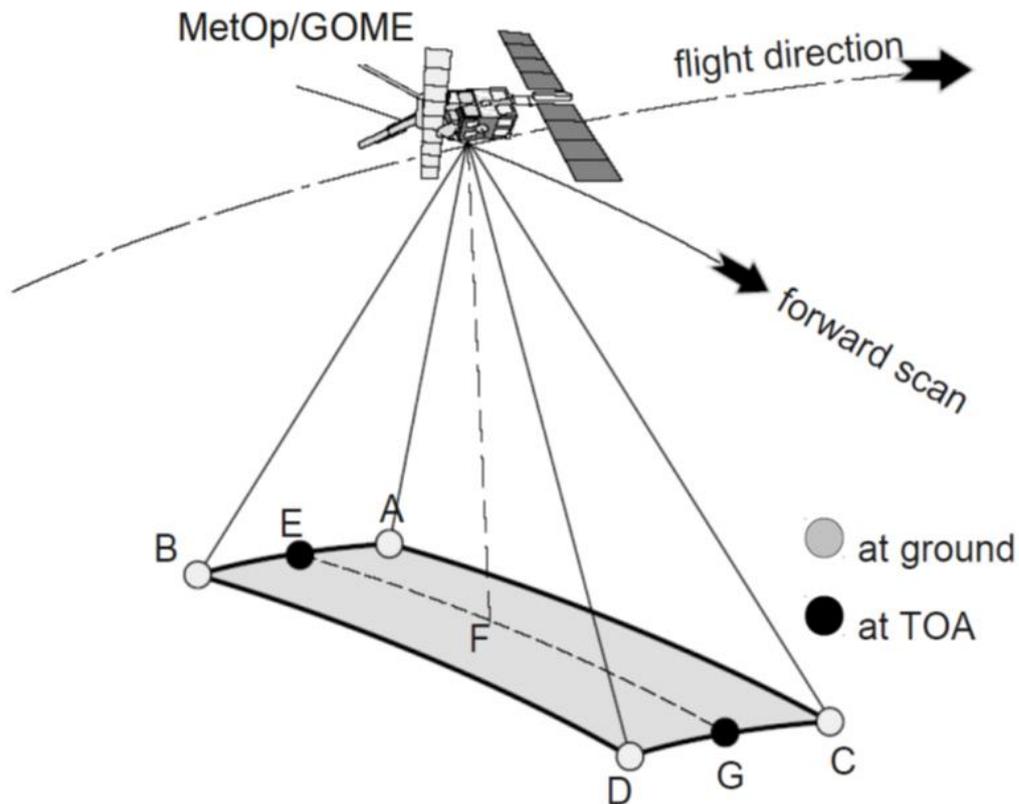


Figure 6: Ground Pixel Geometry

The data sets in the GEOLOCATION group are given in the following table:

Dataset Name	Data Type	Dimension	Unit	Description
corners	string	4	--	dimension variable, order of the corner points
latitude_corners	float	scanline x groundpixel x corners	° North	Latitude of the corner points
longitude_corners	float	scanline x groundpixel x corners	° East	Longitude of the corner points
solar_zenith_angle	float	scanline x groundpixel	degrees	Solar zenith angle at TOA (Point F)

viewing_zenith_angle	float	scanline x groundpixel	degrees	Line-of-sight zenith angle at TOA (Point F)
relative_azimuth_angle	float	scanline x groundpixel	degrees	Relative azimuth at TOA (Point F)

5.5 INPUT_DATA Group

During the data retrieval additional data are read and stored together with the product. The data are necessary for the processing and partly for the interpretation of the Tropospheric BrO columns. An overview of the data is given in the following table:

Dataset Name	Data Type	Dimension	Unit	Description
cloud_fraction	float	scanline x groundpixel	1	Cloud fraction
cloud_top_albedo	float	scanline x groundpixel	1	Cloud top reflectance
cloud_height	float	scanline x groundpixel	km	Cloud height
effective_altitude	float	scanline x groundpixel	km	cloud fraction weighted mean of cloud height and surface height
intensity_weighted_cloud_fraction	float	scanline x groundpixel	1	Cloud fraction
ozone_total_column	float	scanline x groundpixel	DU	Ozone total vertical column
nitrogen_dioxide_stratospheric_column	float	scanline x groundpixel	molec/cm2	nitrogen dioxide stratospheric vertical column
surface_altitude	float	scanline x groundpixel	km	surface altitude
surface_albedo	float	scanline x groundpixel	1	AC-SAF GOME_2 DLER [R5]
surface_condition_flag	int	scanline x groundpixel	1	land-water flag
snow_ice_flag	int	scanline x groundpixel	1	Flag is set if snow cover or ice cover is larger than 20%
tropopause height	float	scanline x groundpixel	km	Tropopause height based on 3.5 PVU and 380K

5.6 Detailed Flag Description

This section gives an overview of all flag datasets. In Sect. 5.6.5 a detailed description on how the flag data can be interpreted can be found.

5.6.1 SwathMode and ViewMode

The SwathMode dataset provides the information about the Swath or Scanning mode of the instrument at the time of acquisition. The information is stored as integer values (see InstrumentMode in Sect. 5.1 for how many ground pixels were observed in the corresponding scanning mode of the instrument view).

Value	Description
0	Nominal
1	Narrow
2	Static
3	SouthPolar
4	NorthPolar

The ViewMode dataset combines the information about the Swath or Scanning mode of the instrument at the time of acquisition (bits 0-7), and the information about the orbital mode (i.e. acquisition during ascending or descending node)

Bit(s)	Value	Description
0-7	0-4	0=Nominal, 1=Narrow, 2=Static Nadir, 3=SouthPolar, 4=NorthPolar
8	256	DescendingFlag Set when ground pixel is in descending part of orbit

5.6.2 surface_condition_flag

These flags give additional information about the surface state during the retrieval. See Sect. 5.6.5 for an example how to use this flag.

Bit	Value	Description
0	0	Land Set when at least 40% of the ground pixel's area is classified as "land"
0	1	Sea Set when at least 60% of the ground pixel's area is classified as "sea"
1	2	Sun glint Set when at least one of the PMD subpixels is affected by sunglint

5.6.3 snow_ice_flag

This flag gives additional information about snow and ice cover. It is updated during the retrieval

Bit	Value	Description
0	0	snow or ice free Set when at least 80% of the ground albedo grid cell (0.25° resolution) is classified as snow or ice free
0	1	snow ice Set when at least 20% of the ground albedo grid cell (0.25° resolution) is classified as snow or ice covered

5.6.4 processing_quality_flag

The QualityFlag dataset provides flags if the measured data is valid. These flags give additional information about the quality of the total column retrieval. Thereby it gives the user an indicator on the limitation of the data set. If for example the fitting of the slant column does not succeed, the flag is set to 1 indicate this condition. If the flag is set to 1 to 8 a fill value is written to the results file.

See MissingDataPercentage in Sect. 5.1 for the percentage of pixels which have been flagged as an overall quality indicator for the whole orbit.

bit	Value	Description
0	0	Valid data
0	1	Invalid column (retrieval failed) e.g. the DOAS retrieval failed BrOTropo contains fill-values
1	2	Large Error in slant column The DOAS retrieval resulted in a RMS larger than 0.04 BrOTropo contains fill-values
2	4	Unfulfilled external dependencies Operational GOME-2 input data had a fill value BrOTropo contains fill-values
3	8	Cloudy conditions Cloud fraction larger than 0.5 BrOTropo contains fill-values
4	16	WARNING Error in slant column The DOAS retrieval resulted in a RMS larger than 0.03 but lower than 0.04 BrOTropo contains data.

Note that if the flag is 16 the data are still valid but the retrieval error is large and the user have to be cautious about the results. This might occur during twilight measurement conditions if the SZA is above 85°.

5.6.5 Flag usage

The flag datasets in the L2 product are stored as binary flags in order to combine different flags in a single dataset. In this way adding further flags in one dataset at a later stage does not affect the dataset itself, so users can still use their routines to read the flag datasets even if new information

was added. In the tables above the integer value of a flag as well as the bit of the flag is given. The integer value can be calculated from $\sum 2^{\text{bit}}$. Here we give an extensive example for the SurfaceConditionFlag dataset (Sect. 5.6.2) in order to explain how to read and interpret these datasets.

In the SurfaceConditionFlag several scenarios can appear: Land/Sea and Sun glint. In principle for a single pixel several scenarios can occur e.g. a pixel over the sea which is subject to sun glint. Represented in binary form it would look like:

0	0	Value		No flag set, i.e. pixel over land, no sun glint
1	0	Bit		
Integer value: 0 (no bit set)				
0	1	Value		Pixel over sea (Land/Sea flag set), no sun glint
1	0	Bit		
Integer value: 1 (2^0 , first bit set)				
1	0	Value		Pixel over land, sun glint (sun glint flag set)
1	0	Bit		
Integer value: 2 (2^1 , second bit set)				
1	1	Value		Pixel over sea, sun glint (both flags set)
1	0	Bit		
Integer value: 3 (2^1+2^0 , first and second bit set)				

In order for a user to check if one of the flags is set the bitwise AND operator has to be used. E.g. in order to check if the sunglint flag bit is set the user has to do the operation 1st bit AND SurfaceConditionFlag(Pixel). Hence the operation would be 2^1 AND SurfaceConditionFlag(Pixel).

As a second example we describe how to use the ViewMode dataset (Sect.5.6.1). This dataset combines two flags within one dataset – first the swath mode of the instrument is stored in the first 8 bits (bits 0-7) and second the information whether it was taken on the ascending or descending node is stored in the 9th bit (bit 8).

In order to filter for a specific swath mode x ($x=0$: nominal, $x=1$: narrow, etc), the first seven bits have to be checked for it i.e. $(2^0+2^1+2^2+2^3+2^4+2^5+2^6+2^7)$ AND ViewMode = x or 255 AND ViewMode = x

To select all pixels from the descending node the user has to check whether bit 8 has been set, i.e. according to our previous example the condition 28 AND ViewMode > 0 must be fulfilled. For the pixels on the ascending node the condition 28 AND ViewMode = 0 applies

Here we give some examples:

Nominal swath, ascending orbit: $(255 \text{ AND ViewMode}) = 0$ & $(256 \text{ AND ViewMode}) = 0$

Nominal swath, descending orbit: $(255 \text{ AND ViewMode}) = 0$ & $(256 \text{ AND ViewMode}) > 0$

Narrow swath, ascending orbit: $(255 \text{ AND ViewMode}) = 1$ & $(256 \text{ AND ViewMode}) = 0$

Narrow swath, descending orbit: $(255 \text{ AND ViewMode}) = 1$ & $(256 \text{ AND ViewMode}) > 0$

Of course the user can also directly check for the integer value of the ViewMode dataset (in the examples above the integer values would be 0; 256; 1; 266, respectively), but if at a later stage the

ViewMode dataset it expanded and more information is stored, then this would affect how the data is filter out by the user's algorithm (e.g. if the user uses all data with ViewMode > 256).

6. USING THE PRODUCTS

This chapter contains practical information on using the GOME-2 tropospheric BrO products.

The data are stored in a two dimensional array 24 ground pixels of the instrument's forward-scan and the scan lines along the track.

6.1 Confidence Flags and Ancillary Fields

The users should check the quality flags (sec 5.6.4) associated with the product. Detailed information is given in the corresponding tables.

6.2 Averaging Kernels

For the tropospheric BrO columns, averaging kernels are provided for each individual GOME-2 pixel. The column averaging kernels A_l are calculated for optically thin absorbers (such as NO₂, HCHO and BrO) as follows:

$$A_l = \frac{m_l}{M_t},$$

where m_l is the altitude-dependent air mass factors for layer l and M_t the tropospheric air mass factor. The tropospheric air mass factor depends on the a priori profile \mathbf{v} via:

$$M_t = \frac{\sum v_l \cdot m_l}{\sum v_l},$$

with v_l being the vertical sub columns of the a priori profile.

Column averaging kernels are essential information on the measurement vertical sensitivity and are particularly useful when comparing measured columns with e.g. model simulations, because they allow removing the effect of the a priori profile shape information used in the retrieval and is required for comparison with other types of data.

The averaging kernels are provided for the model layers of the tropospheric a priori profiles as used in the retrieval (altitude at layer centre). The a priori BrO profiles (in molec/cm³) are also provided in the GOME-2 product, in the following we assume the prior to be given as subcolumns. Combining the information given it should be possible to calculate the tropospheric AMF M_t for any given BrO profile \mathbf{v} e.g. retrieved from MaxDOAS observation.

First the tropospheric AMF M'_t is calculated:

$$M'_t = \frac{M_t \cdot \sum A_l \cdot v'_l}{\sum v'_l}$$

Then the new tropospheric vertical column V'_t is then given by:

$$V'_t = V_t \cdot \frac{M_t}{M'_t}$$

6.3 Software and Tools for reading the products

The netCDF products can be read using the standard netCDF4 software and tools available at:

<https://unidata.github.io/netcdf4-python/netCDF4/index.html>

NASA offers the netcdf data viewer panoply for download at:

<https://www.giss.nasa.gov/tools/panoply/>