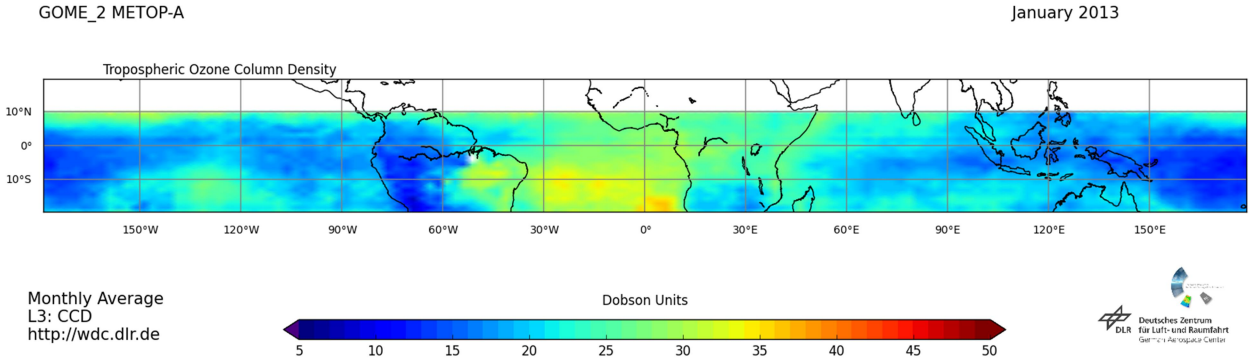
Product user manual for Tropospheric Ozone Columns retrieved from GOME-2 / GOME data

Deutsches Zentrum für Luft- und Raumfahrt
German Aerospace Center



Signatures

Action: Name	*Affiliation*	*Function*	*Date*	*Sign.*
prepared by:				
P. Valks	DLR-MF	AC SAF Project Manager		
D. Loyola	DLR-MF	GOME Project Manager		
K-P. Heue	DLR-MF	GOME Project Scientist		
W. Zimmer	DLR-MF	GOME Project Scientist		
released by:				
P. Valks	DLR-MF	AC SAF Project Manager		

Document change log

Issue / Rev	Sections	changes	Date
0	All	--	Sep.2014
0.1	All	Description of the algorithm PUM for GOME_2 only	1 Oct. 2014
0.2	All	PUM for both GOME_2 and GOME_1 add EUMETSAT O3M-SAF project, minor corrections, clarifications	16 Oct. 2014
0.9	All	Data organisation and filename similar to level2 data	10 Feb. 2015
1 / A	All	Minor corrections	10 June 2015
1 / B	All	Update including GOME-2C	4 Feb.2020

Internal product ID's for project control

Product	***Instrument***	***Product ID***
Offline Tropical Tropospheric Ozone	GOME-2/MetOp-A	O3M-35
Offline Tropical Tropospheric Ozone	GOME-2/MetOp-B	O3M-43
Offline Tropical Tropospheric Ozone	GOME-2/MetOp-C	O3M-302

Table of Contents

1. Introduction

Purpose and scope

DLR produces GOME/ERS-2 and GOME-2/MetOp-A, B and C tropospheric ozone products operationally in the framework of the projects EUMETSAT AC-SAF.

Based on the GOME-2 and GOME 1 operational ozone column and cloud level 2 products [R1, R2] an algorithm has been developed to retrieve tropospheric ozone columns in tropics. This algorithm applies the convective cloud differential (CCD) method to retrieve tropospheric ozone columns. This document is the user manual for the GOME /GOME-2 tropospheric ozone column (level 3 product).

In this document, the terms GOME/ERS-2 and GOME-2/MetOp-A, GOME-2/MetOp-B or GOME-2/ MetOp-C are used to reference the specific instruments. The general term GOME applies to all three sensors.

Abbreviation and Acronyms

AMF	Air Mass Factor
ccd	convective cloud differential (method to retrieve the tropospheric column)
DLR	Deutsches Zentrum für Luft- und Raumfahrt (german aerospace centre)
ERS-2	European Remote Sensing Satellite 2
GDP	GOME Data Processor
GOME	Global Ozone Monitoring Experiment
GOME-2	Global Ozone Monitoring Experiment 2
MetOp (A, B)	Operational Metrological Satellite (A or B)
netCDF	network Common Data Format
OCRA	Optical Cloud Recognition Algorithm
PMD	Polarisation Measurement Device
RMS	Root Mean Square
ROCINN	Retrieval of Cloud Information using Neural Networks
SCD	Slant Column Density

2. Description of the algorithm

Introduction

The tropospheric ozone retrieval is based on the GOME ozone columns as derived by the GOME Data Processor (GDP). The GDP uses an optimized DOAS fit to retrieve slant column densities (SCD) of several trace gases from the measured spectra. The ozone SCD fit is performed in a fitting window between 325 and 335 nm. 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 and in the

calculation of the tropospheric ozone column is obtained with the OCRA and ROCINN algorithms. A detailed description of the GDP algorithms is given in [R1], [R3] [R5] [R6] and [R7].

Tropospheric ozone retrieval

The convective cloud differential algorithm is described in detail in [R1] [R3] and [R8]. The retrieval uses the level 2 data product as input. The stratospheric column is approximated by the ozone column above high reaching convective clouds. The level 2 ozone columns are filtered for high reaching convective clouds with high cloud fraction and cloud albedo. After dividing the data by the above cloud AMF the monthly averaged and gridded data define the local stratospheric column [SUPPORT_DATA/ DETAILED_RESULTS/STRATOSPHERIC_OZONE/stratospheric_O3]. Because the stratospheric ozone only shows a weak longitudinal dependency the average stratospheric column in a reference region between the eastern Indian Ocean and the western Pacific (70°E eastwards to 170°W) is used for each latitude band [SUPPORT_DATA/DETAILED_RESULTS/STRATOSPHERIC_OZONE/stratospheric_O3_reference].

The total columns in the cloud free GOME pixels contain the complete tropospheric signal in addition to the stratospheric one. Therefore the difference between the total ozone columns [SUPPORT_DATA/ DETAILED_RESULTS/TOTAL_OZONE/total_O3] for cloud free observations and the stratospheric column for the respective latitude band equals the tropospheric column [PRODUCT].

The data are gridded to a 1.25° x 2.5° grid for GOME-2 and 2.5° x 5° for GOME/ERS-2 and averaged over a certain time period (e.g. 1 month).

3. Data format

The data are stored in the netCDF-4 format. An overview of the “METADATA” together with a short description and possible values is shown in Table 3-1. The METADATA are attributes of the group: “METADATA/O3MSAF_METADATA” The longitude / latitude grid defines the two dimensions listed in Table 3-2. The variables’ short names are listed in Table 3-4 to Table 3-8. The data are stored in the “PRODUCT” group, containing the main product, and the subgroups in “SUPPORT_DATA/ DETAILED_RESULTS” containing ancillary products, which were calculated during the data processing.

Table 3-1: List of global attributes, typical values, and a short description.

Attribute	possible values	Description
Conventions	CF-1.6	Climate and Forecast convention for variable names, units and dates
filename	GOME_(1,2)_tropO3_ Tropics_YYYYMM_1Month_plat-form (ERS, METOP-A, METOP-B,METOP-C)_DLR_version .nc	The filename starts with the sensor name, followed by the content (tropO3_Tropics), the year and the month and the time period used for this product (1Month), than the platform (e.g. METOP-A), the institution (DLR) before it ends with a version number

institution	DLR Deutsches Zentrum fuer Luft und Raumfahrt	Institution, responsible for the data
reference	http://atmos.eoc.dlr.de/gome/gto-ecv.html	
creator_name	Klaus-Peter Heue	responsible for the data
creator_email	Klaus-Peter.Heue@dlr.de	contact address
processing_time	YYYY-MM-DDTHH:mm:ssZ	date and time (UTC) when this file was created, CCSDS format
base_product	Level2 GDP	basis of this data product
base_productVersion	4.6 – 4.9	version of the underlying data
product_algorithm_name	CCD-trop	
product_algorithm_version		version of this data product
product_format_type	NetCDF	file type
product_format_version	4	type version
product_content	Tropospheric_Ozone, Stratospheric_Ozone, Total_Ozone, Cloud_Parameters, Surface_Properties	short description of the file content
project	EUMETSAT O3M-SAF	
geospatial_latitude_min	-20	minimum latitude (20°S)
geospatial_latitude_max	20	maximum latitude (20°N)
geospatial_latitude_resolution	1.25 / 2.5[1]	resolution for GOME-2 and GOME
geospatial_latitude_units	Degrees_North	unit of the latitude
geospatial_longitude_min	-180	minimum longitude (180°W)
geospatial_longitude_max	180	maximum longitude (180°E)
geospatial_longitude_resolution	2.5 / 5	resolution for GOME-2 and GOME
geospatial_longitude_units	Degrees_East	unit of the longitude
geospatial_vertical_range_bottom_troposphere	surface	minimum altitude for the tropospheric column product
geospatial_vertical_range_top_troposphere	10-14	maximum altitude for the tropospheric column product
geospatial_vertical_range_bottom_stratosphere	10-14	minimum altitude for the stratospheric column data
geospatial_vertical_range_top_stratosphere	80	maximum altitude for the stratospheric column data
geospatial_vertical_range_bottom_total	surface	minimum altitude for the total column data
geospatial_vertical_range_top_total	80	maximum altitude for the total column data
geospatial_altitude_unit	km	unit of the altitude data
time_coverage_start	YYYY-MM-DD	first day of measurement period

[1] The grid resolution depends on the sensor, for GOME-2/MetOp it is 1.25 x 2.5°, for GOME/ERS-2 it is 2.5° x 5°

time_coverage_end	YYYY-MM-DD	last day of measurement period
sensor	GOME-2 / GOME	sensor name
platform	METOP-A/B/C / ERS-2	satellite
projects	AC-SAF	project the data belong to
product_ID	O3M – XXX	Product identifier, as given in O3MSAF Product Requirement Document

Table 3-2: Overview of the dimension in the data file.

Dimension name	Unit	Size	Description
Latitude	Degree north (-20, 20)	32 / 16[1]	1.25° / 2.5° latitudinal resolution
Longitude	Degree east (-180, 180	144 / 72	2.5° / 5° longitudinal resolution

Table 3-3: Overview of the variables associated to the dimensions

Variable name	Unit	Size	Description
Latitude	Degree north	32 x 144 / 16 x 72 f32[2]	Centre of the gridded data
Longitude	Degree east	32 x 144 / 16 x 72 f32	Centre of the gridded data

Table 3-4: Overview of the variables in the product group.

Besides the tropospheric ozone column between 20°N and 20°S the product group contains a subgroup SUPPORT_DATA, where many auxiliary data are stored. The variables "tropospheric_O3_xx" have two attributes describing the data's altitude range, vertical_range_bottom (=surface) and vertical_range_top.

Variable name	Unit	Size	Description
tropospheric_O3	DU	32 x 144 / 16 x 72 f32	averaged tropospheric ozone column
tropospheric_O3_ mixingratio	ppb	32 x 144 / 16 x 72 f32	averaged tropospheric ozone mixing ratio
tropospheric_O3_std	DU	32 x 144 / 16 x 72 f32	standard deviation of the tropospheric ozone columns
tropospheric_O3_ mixingratio_std	ppb	32 x 144 / 16 x 72 f32	standard deviation of the tropospheric ozone mixing ratios
tropospheric_O3_ number	-[3]	32 x 144 / 16 x 72 int	Number of individual observations
SUPPORT_DATA/DETAILED_RESULTS			
STRATOSPHERIC_OZONE		Table 3-5	
TOTAL_OZONE		Table 3-6	
CLOUD_PARAMETERS		Table 3-7	
SURFACE_PROPERTIES		Table 3-8	

a. STRATOSPHERIC_OZONE subgroup

In the tropospheric ozone retrieval in a first step the stratospheric vertical column is calculated. The data for each grid cell as well as for the stratospheric reference region are given in this subgroup. The altitude range for all the data in this subgroup is given as group attributes: vertical_range_bottom and vertical_range_top (80 km).

[2] The standard data type is float using 32 bit precision (f32) or integer (int) for natural numbers and flags
[3] In the file unit "1" is used, to be conform with the cf-conventions.

Table 3-5: Variable names in the stratospheric Ozone subgroup

Variable name	Unit	Size	Description
stratospheric_O3	DU	32 x 144 / 16 x 72 f32	average stratospheric ozone columns
stratospheric_O3_std	DU	32 x 144 / 16 x 72 f32	standard deviation of the stratospheric ozone column
stratospheric_O3_number	-	32 x 144 / 16 x 72 f32	number of individual observations
stratospheric_O3 _reference	DU	32 / 16 f32	average stratospheric ozone column in the reference area
stratospheric_O3 _reference_std	DU	32 / 16 f32	standard deviation of the stratospheric ozone column in the reference area
stratospheric_O3 _reference_number	DU	32 / 16 int	number of individual observation in the reference area
stratospheric_O3 _reference_flag	-	32 / 16 int	see flag description Table 3-9

b. TOTAL_OZONE subgroup

During the analysis the total columns for the cloud free pixels are averaged. The altitude range for these data stretches from vertical_range_bottom(=surface) to vertical_range_top(=80 km)

Table 3-6: Total ozone variables

Variable name	Unit	Size	Description
total_O3	DU	32 x 144 / 16 x 72 f32	average total ozone columns
total_O3_std	DU	32 x 144 / 16 x 72 f32	standard deviation of the total ozone
total_O3_number	-	32 x 144 / 16 x 72 int	number of individual observations

c. CLOUD_PARAMETERS subgroup

The stratospheric data are calculated from ozone columns above high clouds. Here only observations with high reaching clouds (CTH>10km), high cloud fraction (f>0.8) and cloud albedo (a>0.8) are used. For these three parameters the average values and the standard deviations are given. The number of individual observation is not given here, because it is the same as for the stratospheric ozone column

Table 3-7: average cloud parameters used for the stratospheric column retrieval

Variable name	Unit	Size	Description
cloud_albedo	-	32 x 144 / 16 x 72 f32	average cloud albedo
cloud_albedo_std	-	32 x 144 / 16 x 72 f32	standard deviation of the cloud albedo
cloud_fraction	-	32 x 144 / 16 x 72 f32	average cloud fraction
cloud_fraction_std	-	32 x 144 / 16 x 72 f32	standard deviation of the cloud fraction
cloud_height	km	32 x 144 / 16 x 72 f32	average cloud height
cloud_height_std	km	32 x 144 / 16 x 72 f32	standard deviation of the cloud height

d. SURFACE_PROPERTIES subgroup

The surface properties from the level 2 data (cloud free observations) are averaged to the resolution of the level 3 product. No standard deviation is given.

Table 3-8: description of the surface properties.

Variable name	Unit	Size	Description
surface_albedo	-	32 x 144 / 16 x 72 f32	average surface albedo
surface_flag	-	32 x 144 / 16 x 72 f32	land sea flag Table 3-10
surface_height	km	32 x 144 / 16 x 72 f32	average surface height

e. Flag description

Before subtracting the stratospheric reference column from the total column the stratospheric data are quality checked. The stratospheric reference column might be classified as invalid for the reasons given in the table below. In these cases no tropospheric O_3 column is calculated for the entire latitude band. However, there are two exceptions focussing on outlier cases where one stratospheric reference column is classified different from the two neighbouring ones:
If the data number of data is low, but the stratospheric reference column agrees well with the neighbouring reference columns and they are not classified as invalid and the tropospheric column will be given anyway.
If two stratospheric reference columns are classified as invalid data and only one column in between is classified as valid, no tropospheric columns are given for the single remaining band.

In case data are flagged for more than one reason, the flag values are added.

Table 3-9: Quality flag for the stratospheric reference data

Flag value	Description	Threshold
0	valid stratospheric reference data	
1	stratospheric ozone column out of range	< 200 DU
2	number of individual observations too low	< 18 / 8[4] measurements per latitude band
4	standard deviation too high	> 10 DU
8	latitudinal gradient in stratospheric ozone too large	> 3.6 /4.2 DU difference between two neighbouring latitude bands, both will be flagged

[4] The values of these two thresholds varies with the sensor the first number belongs to GOME_1 the second one to GOME_2.

The surface flag gives additional information about the surface condition. The surface data are distinguished between land, sea and coast. The product is based on the land / sea flag of the GOME Level 2 product. The coastal flag was introduced to consider small landmasses (e.g. Hawaii or parts of Indonesia) in the coarse resolution (1.25° x 2.5° / 2.5° x 5°) of the level 3 product.

Table 3-10 Land / sea flag

Flag value	Description	Threshold
0	Land	if less than 20 % of all GOME-2 /GOME level 2 observations were classified as sea
1	Coast	between 20% and 80% were classified as sea
2	Sea	more than 80% were classified as sea

4. References

[R1] P. Valks, D. Loyola, N. Hao, P. Hedelt, S. Slijkhuis, M. Grossi, Algorithm Theoretical Basis Document for GOME-2 Total Column Products of Ozone, Tropospheric Ozone, NO_2, tropospheric NO_2, BrO, SO_2, H_2O, HCHO, OClO, and Cloud Properties (GDP 4.7 for O3M-SAF OTO and NTO), DLR/GOME- 2/ATBD/01, Iss./Rev. 2/F, 28 June 2013.

[R2] Product User Manual for GOME Total Columns of Ozone, NO_2, tropospheric NO_2, BrO, SO_2, H_2O, HCHO, OClO, and Cloud Properties, DLR/GOME/PUM/01 28 June 2013

[R3] P. Valks, K.-P. Heue, D. Loyola, N. Hao: Algorithm Theoretical Basis Document for GOME-2 tropical tropospheric Ozone Column Products DLR/GOME-2/ATBD_toc/01, Iss./Rev. 1/A, Oct 2014.

[R4] R. Spurr, M. van Roozendael, D. Loyola, C. Lerot, J. van Geffen, J. van Gent, C. Fayt, J.-C. Lambert, W. Zimmer, A. Doicu, S. Otto, D. Balis, M. Koukouli, C. Zehner, GDP 5.0 Upgrade of the GOME Data Processor for Improved Total Ozone Columns — Algorithm Theoretical Basis Document, DLR/GOME/ATBD/GDP5, Iss./Rev. 1B, August 2012.

[R5] Algorithm Theoretical Basis Document for GOME Total Column Densities of Ozone and Nitrogen Dioxide, UPAS/GDOAS: GDP 4.0, ERSE-DTEX-EOPG-TN-04-0007, Iss./Rev. 1/A, December 2004.

[R6] Hao, N., Koukouli, M. E., Inness, A., Valks, P., Loyola, D. G., Zimmer, W., Balis, D. S., Zyrichidou, I., Van Roozendael, M., Lerot, C., and Spurr, R. J. D.: GOME-2 total ozone columns from MetOp-A/MetOp-B and assimilation in the MACC system, Atmos. Meas. Tech., 7, 2937-2951, doi:10.5194/amt-7-2937-2014, 2014.

[R7] Loyola, D. G., Koukouli, M. E., Valks, P., Balis, D. S., Hao, N., Van Roozendael, M., Spurr, R. J. D., Zimmer, W., Kiemle, S., Lerot, C., and Lambert, J.-C.: The GOME-2 total column ozone product: Retrieval algorithm and ground-based validation, J. Geophys. Res., 116, D07302, doi: 10.1029/2010JD014675, 2011

[R8] Valks, P., Hao, N., Gimeno Garcia, S., Loyola, D., Dameris, M., Jöckel, P., and Delcloo, A.: Tropical tropospheric ozone column retrieval for GOME-2, Atmos. Meas. Tech., 7, 2513-2530, doi: 10.5194/amt-7-2513-2014, 2014.